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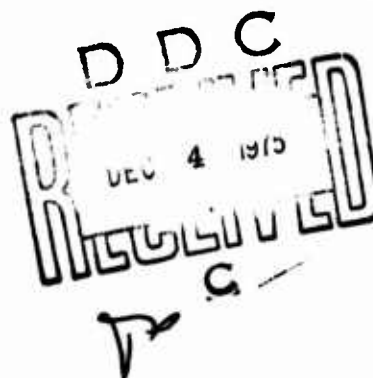
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CONTRACT REPORT NO. 265

**TWOFLO - A COMPUTER CODE TO SOLVE THE
PROBLEM OF TWO-PHASE FLOW WITH SHOCKS
IN A DUCT**

Prepared by

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October 1975

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NOMENCLATURE

- A = bulk sound speed of gas
 A_B = cross sectional area of the bullet
 c = cross-sectional area of duct
 C_p = constant pressure specific heat of the gas
 C_v = constant volume specific heat of the gas
 D_b = barrel diameter
 D_c = chamber diameter
 E = internal energy of gas per unit mass of gas
 \hat{E} = internal energy of combustion products per unit mass of gas
 E_p = internal energy of particle per unit mass of particle
 E_w = internal energy of gas per unit mass of gas leaving through the wall
 E_{wp} = internal energy of particle unit mass of particle leaving through the wall
 F = force per unit volume of mixture resulting from gas acting on particle (positive when acting in positive x direction)
 F_R = bore resistance force
 F_w = wall friction force on gas per unit volume of mixture (positive when acting in positive x direction)
 F_{wp} = wall friction force on particle per unit volume of mixture (positive when acting in positive x direction)
 H = enthalpy of gas
 K_n = particle's velocity ratio across area discontinuity
 K_Q = amount of heat released per unit volume of propellant burnt
 L_B = bullet length
 L_{BR} = barrel length (measured from where barrel diameter begins to muzzle)
 L_p = length of cylindrical portion of particle
 M_B = mass of the bullet
 M_p = mass of a single particle
 N = number of particles per unit volume of mixture
 N_g = number of particles per unit mass of gas

P = pressure of gas (also equal to pressure of mixture)
 P_{AFT} = pressure immediately after the bullet
 P_{BEF} = pressure immediately behind the bullet
 P_{BEX} = pressure behind the bullet immediately before it leaves the barrel
 P_d = nondimensionalizing pressure
 P_{EXIT} = pressure behind shock when it leaves the barrel
 P_h = hold back pressure
 P_M = muzzle pressure (usually atmospheric pressure)
 P_w = pressure of the gas leaving through wall perforations
 q = time rate of heat addition to gas per unit mass of gas from internal sources
 q_p = time rate of heat addition to particles per unit mass of particle from internal sources
 q_w = time rate of heat addition to gas per unit mass of gas from duct wall
 q_{wp} = time rate of heat addition to particles per unit mass of particle from duct wall
 Q = rate at which total energy is added to the gas per unit volume of mixture due to burning
 Q_p = rate at which total energy is added to the particle phase per unit volume of mixture due to burning
 Q_p^* = total heat released by a propellant particle from ignition to time t .
 Q_w = rate at which total energy is added to the gas phase per unit volume of mixture due to mass transfer through wall perforations
 Q_{wp} = rate at which total energy is added to the particle phase per unit volume of mixture due to mass transfer through wall perforations
 R_p = particle radius
 S = entropy of gas
 S_p = burning surface
 t = time
 t_{BD} = time that it takes for P_{BEX} to reach P_M after bullet leaves the barrel
 t_{EX} = time that bullet leaves the barrel
 t_{SD} = time that it takes for P_{EXIT} to reach P_M after shock leaves the barrel
 T = temperature of gas
 T_w = wall temperature
 u = velocity of gas
 u_p = velocity of particle

u_w = velocity of gas leaving through the wall in the x direction
 u_{wp} = velocity of particle leaving through the wall in the x direction
 U = shock velocity
 v_w = velocity of gas leaving through the wall in the radial direction
 v_{wp} = velocity of particle leaving through the wall in the radial direction
 V_B = volume of a propellant particle burnt from ignition to time t
 V_p = volume of a propellant particle remaining at time t
 x = position coordinate along axis of duct (positive from breech to muzzle)
 x_{BAR} = x location where barrel diameter begins
 x_B = x location of bullet
 x_C = x location where chamber diameter ends
 x_d = nondimensionalizing length
 x_M = x location of muzzle
 Z = regression distance
 α = constant in regression formula
 β = constant in regression formula
 γ = ratio of specific heat C_p/C_v
 c = volume fraction of particle
 μ = dynamic viscosity
 ρ = density of gas = mass of gas per unit volume of gas
 ρ_d = nondimensionalizing density
 ρ_p = density of particles = mass of particles per unit volume of particles
 ρ_w = density of gas leaving through the wall
 σ = gas concentration (mass of gas per unit volume of mixture)
 σ_p = particle concentration (mass of particles per unit volume of mixture)
 ϕ = the rate at which work is done on the gas per unit mass of gas from all forces

I. INTRODUCTION

This document is a final contract report for contract DAAD05-74-C-0749. The research under this contract is aimed toward the development of a computer code which utilizes the method of characteristics to solve the problem of two-phase flow with shocks. This type of flow is typical of flow in a projectile launch tube, where combustion products and unburnt propellant grains are mixed. Usually, this complicated flow, which may contain shocks of relatively large amplitude, is approximated either by a pure gas flow or by a simplified two-phase flow model where the gas and particles have the same or predetermined relative velocities. A better model to handle this problem is required to test the accuracy of simplified formulations and to produce a more accurate prediction of the flow, particularly in the presence of shocks.

In addition to presenting the general formulation, a discussion of the proper initial-boundary values to be prescribed for the present mixed hyperbolic-parabolic equations is presented. It is shown that there is a region immediately behind the bullet in which only the gas phase is present. This consideration requires the development of an interface between a one-phase and two-phase region. The computer code TWOFLO which utilizes the method of characteristics and finite difference techniques to solve the problem of a projectile accelerating in a gun barrel is presented.

1. State of the Art

Quite a few textbooks and manuals, such as, Corner [1], Hunt [2] and the Army Design Handbook [3] exist in the field of internal ballistics; however, most of these works give only qualitative descriptions, or present simple experimental results. They are not sufficient for modern design application; more up-to-date computer codes are needed to better model the internal ballistics problem.

In recent years, computer codes have been developed to treat the internal ballistics problem. Examples of which are codes written by Baer and Frankle [4] and Baer [5]. These codes for the most part are limited in that they are restricted to one-phase flows where the particle motion is predetermined. This is satisfactory when the particles are very small, and the loading ratio is low, thus the particles and the gas are in equilibrium. However, for problems where finite size propellant particles are packed with a high loading ratio, the motion of the particles is different from that of the gas and the flow should be treated as two distinct phases. In 1956, under BRL sponsorship, a group at the University of Maryland discussed the equations of two-phase flow and proposed schemes for numerical calculation; however no attempt was made to write a code [6]. Other works such as Refs. [7] and [8] are only for special applications, with various limitations and simplifications.

There is a need for an up-to-date two-phase flow code that will trace shock waves exactly, handle high loading ratios, include the effects of finite particle volume, accommodate a general form of the equation of state and various other features. With today's high speed computers and the knowledge of numerical methods, it is feasible to develop such a code.

To solve this problem numerically either a two-dimensional or a one-dimensional code may be developed. As discussed by Moretti [9] two-dimensional codes are certainly more versatile; however, for certain problems, the results of two-dimensional codes are often less than satisfactory, with uncertainties in convergence, stability and physical meaning. On the other hand, one-dimensional codes can be used more conveniently for studying the importance of different parameters and for delineating the physical nature of the problem. In view of the present state-of-the-art in two-phase flow, a one dimensional code would be most useful to solve interior ballistic problems.

In this report, we present a one-dimensional two-phase flow code, in which a shock wave is traced exactly both in front of and behind the projectile. In continuous regions, we shall use the basic method of characteristics supplemented by finite-difference techniques in places where characteristics do not exist. The method of characteristics has the advantage that it reveals more directly the flow properties and wave structure.

2. General Features of the Code

The following are some of the features that are included in the final code.

- a. The computer code is written in such a way that any consistent set of units can be used.
- b. The code is written in FORTRAN IV language.
- c. Provisions have been made to account for heat loss through the barrel, wall friction, and mass loss through holes in the barrel.
- d. The code is designed to handle gradual changes in bore area.
- e. The code does not handle ignition; therefore, all propellant particles will be assumed to be ignited before calculations begin. An ignition code must be used to generate the initial conditions $p(x,0)$, $\epsilon(x,0)$, $\rho(x,0)$, $\rho_p(x,0)$, $z(x,0)$, $u(x,0)$ and $u_p(x,0)$ which will be substituted into the present code. A shock wave may be present initially.
- f. The bore resistance is treated as a function of x , u and Δp .
- g. The gas in front of the bullet is treated including the possible formation of a shock.
- h. A single shock wave can automatically be inserted and traced behind the projectile.
- i. The barrel configuration is of the form shown in Fig. (1).

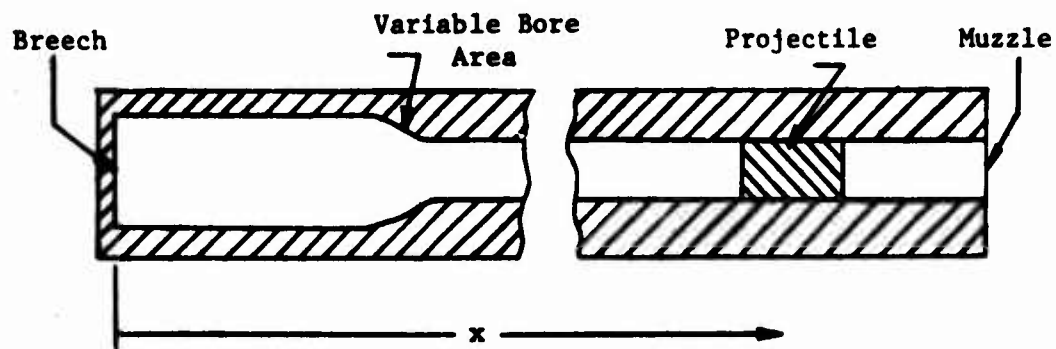


Figure 1 - Schematic Barrel Configuration

II. GENERAL FORMULATION

1. Literature Review

The problem of two-phase flow has drawn considerable attention in recent years. This interest is stimulated mostly by applications such as solid propellant rockets, nuclear reactors, fuel sprays, lunar ash flow and, of course, interior ballistics. The governing equations of two-phase flow have been presented by many authors. A few of these will be discussed here.

Rudinger [10, Section 4] derived a set of equations for solid particles suspended in a gas where the particle volume fraction is finite. A simpler set of equations neglecting the particle volume was also presented [10, Section 7]. This simple set of equations was solved numerically for an unsteady flow problem [11]. Rudinger gave detailed physical meaning to various terms in his equations and discussed the shock conditions and relaxation times. His formulation is not suitable for direct application to the present problem, because (a) it is limited to an ideal gas equation of state, (b) no mass transfer between the particle and the gas is considered, (c) no transport of mass, momentum, and energy between the mixture and the duct wall is allowed, (d) no provision is made for a change of duct area along the axis, and (e) the pressure gradient force on the particle is neglected.

Migdal and Agosta [12] derived two-phase flow equations by considering the particle terms as a source of drag and heat transfer in a pure gas flow. They included the effects of mass, momentum and energy transport between the particles and the gas, without giving explicit expressions for them and limited their study to the case of small particle volume. Using concepts in continuum mechanics, such as partial stress and partial energy, Soo [13] derived equations for multiphase flow. He emphasized the importance of the size distribution of the solid particles, and wrote a set of fundamental equations treating solid particles of different sizes as distinct species in the mixture. This approach is not directly suitable for practical application because in general the size distribution of the solid particles is more or less continuous. Panton [14] treated the two-phase flow problem by defining all physical quantities in terms of their time and spacial averages. This approach may be suitable for a turbulent flow study, but is too cumbersome for other purposes. Murray [15] derived a set of equations to be used primarily for fluidization applications. He assumed a constant particle volume ratio and neglected pressure forces acting on the particles. In each of his equations of motion terms involving the time derivative of both the fluid and particle velocities are included. As will be shown later, these terms will change the nature of the governing equations. Marble [16] also applied modern techniques of fluid mechanics to the two-phase flow problem of a gas and solid particles, however, he limited his study to the case of a negligibly small particle volume fraction.

Most studies of a two-phase flow are limited to the case of a negligibly small particle volume fraction. As mentioned before, Rudinger [10] included the volume fraction terms, but did not consider the pressure gradient force acting on the particle. Pai [17] included the particle volume fraction term and also the pressure gradient force. He treated this pressure force by considering the particles as a pseudo-fluid with a partial pressure. This pseudo-fluid, however, does not contribute to the pressure of the mixture. In doing this, the term containing the spacial derivative of the particle volume fraction, $\frac{\partial \epsilon}{\partial x}$, was not included. For problems where ϵ is not negligible the derivative may be of the same order as other terms in the equations and its omission may cause appreciable error.

In this report, we derive the governing equations including the pressure gradient force on the particles, and also the $\frac{\partial \epsilon}{\partial x}$ term. It will be shown that the inclusion of this term causes the characteristic properties of the equations to change. When this term is neglected, two compatibility equations exist along the triple degenerate characteristic, $\frac{dx}{dt} = u_p$, while when it is included, only one exists (for further details see Sec. III,1)

2. Basic Assumptions

The governing equations are derived on the basis of the following assumptions:

- a. The equation of state of the gas is of the form $p=p(\rho, E)$ or $p=p(\rho, T)$.
- b. The average size of the actual particles will be used in the equations; they are incompressible; their specific heat is constant, and the temperature is uniform within each particle.
- c. The particles are uniformly distributed over the cross-section of the duct, and their size and average spacing are small compared with the cross-sectional area.
- d. The flow is treated as one-dimensional, thus changes in the cross-sectional area of the duct must be sufficiently gradual. Abrupt changes in the cross-sectional area must be treated by matching the continuous flow regions on both sides.
- e. The drag force between the gas and particle phases is assumed known. It may be prescribed as a function of any of the flow variables. The modified Stokes formula and Ingebo formula, which were used by Pai and Rudinger, are typical drag force expressions.
- f. The effect of the particles on the gas flow is distributed over the entire gas phase by mixing. This mixing involves only a small gas volume and is therefore assumed to take place instantaneously.

- g. The size of the particles to be considered will be a few orders of magnitude larger than the molecules of the gas. It will be assumed, therefore, that the particles do not contribute to the pressure of the mixture. The pressure of the gas-particle mixture is given by the pressure in the gas phase alone. The volume fraction of the particles, ϵ , will not be assumed small. Therefore, the pressure gradient will act on the particles, as well as on the gas, and will be included in the momentum equations of the particles.
- h. Gravitation and other body forces will not be included in the equations.
- i. The density ratio between the particles and the gas is small enough so that terms containing ρ/ρ_p may be dropped from the equations.
- j. The particle density ρ_p is constant.

3. Governing Equations

Under these assumptions, the governing equations for the gas medium are (for a detailed derivation see Appendix A) the continuity equation,

$$\frac{D\sigma}{Dt} + \sigma \frac{\partial u}{\partial x} = - \frac{\sigma u}{A} \frac{dA}{dx} + \omega - \omega_w \quad (1)$$

the momentum equation,

$$\frac{Du}{Dt} + \frac{(1-\epsilon)}{\sigma} \frac{\partial p}{\partial x} = - \frac{1}{\sigma} [(F-F_w) - \omega(u_p-u) + \omega_w(u_w-u)] \quad (2)$$

and the energy equation

$$\begin{aligned} \frac{DE}{Dt} + \frac{p}{\rho} \frac{\partial u}{\partial x} - \frac{pu}{\sigma} \frac{\partial \epsilon}{\partial x} = \frac{1}{\sigma} [Q+Q_w + u(F-F_w) - Fu_p - \omega(uu_p - \frac{1}{2} u^2 + E) \\ + \omega_w(uu_w - \frac{1}{2} u^2 + E) - \omega_{wp} \frac{p}{\rho_p} - \frac{pu(1-\epsilon)}{A} \frac{\partial A}{\partial x}] \end{aligned} \quad (3)$$

The governing equations for the particles are the continuity equation

$$\frac{D^p \sigma}{Dt} + \sigma_p \frac{\partial u}{\partial x} = - \frac{\sigma_p u}{A} \frac{dA}{dx} - \omega - \omega_{wp} \quad (4)$$

the momentum equation,

$$\begin{aligned} \frac{D^p u}{Dt} = \frac{1}{\sigma_p} \left\{ \frac{\epsilon}{1-\epsilon} [(F-F_w) - \omega(u_p-u) + \omega_w(u_w-u)] \right. \\ \left. + (F + F_{wp}) - \omega_{wp}(u_{wp}-u_p) \right\} \end{aligned} \quad (5)$$

and the energy equation, which is uncoupled from the system,

$$\begin{aligned} \frac{D^p E}{Dt} + \frac{p}{\rho_p} \frac{\partial u}{\partial x} + \frac{pu}{\sigma_p} \frac{\partial \epsilon}{\partial x} = \frac{1}{\sigma_p} [Q_p + Q_{wp} \\ + u_p F_{wp} + (E_p + \frac{u_p^2}{2})(\omega + \omega_{wp}) - \frac{\epsilon p u}{A} \frac{\partial A}{\partial x}] \end{aligned} \quad (6)$$

where D/Dt and D^P/Dt are material derivatives of the gas and particle properties, respectively, and are given by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x}$$

and

$$\frac{D^P}{Dt} = \frac{\partial}{\partial t} + u_p \frac{\partial}{\partial x}$$

Equations (1)-(6) represent a system of 6 equations in terms of 8 unknowns σ , u , E , p , σ_p , u_p , E_p and ϵ . To complete this system we must supply the equation of state of the gas

$$p = p(\rho, E) \quad (7)$$

and the definitions of σ and σ_p

$$\sigma = (1-\epsilon)\rho \quad (8)$$

and

$$\sigma_p = \epsilon \rho_p \quad (9)$$

With the assumption that ρ_p is constant (the particle is incompressible), Eqs. (1)-(9) represent a system of 9 equations in terms of 9 unknowns σ , u , E , ρ , p , ϵ , σ_p , u_p , and E_p . The terms ω , ω_w , ω_{wp} , F , F_w , F_{wp} , Q , Q_p , Q_w , and Q_{wp} appearing on the right hand side of Eqs. (1) to (9) will be considered as given input information; they may be either functions of x and t , or functions of the flow properties. Usually, they do not contain derivatives of the flow properties with respect to x or t ; therefore they will not affect the characteristic directions and the form of compatibility equations associated with the system.

4. Initial and Boundary Conditions

When attempting to determine a set of properly posed initial and boundary conditions for a set of equations, it is beneficial to have a thorough understanding of their characteristic directions and compatibility equations, since the two are closely related. The details concerning the characteristics associated with Eqs. (1)-(5) can be found in Sec.(III,1); however, a few pertinent observations will be presented here.

First, the particle phase equations, Eqs. (4) and (5), are weakly coupled to the gas phase equations, Eqs. (1), (2) and (3) (note that the converse is not true), thus the characteristic directions associated with each phase can be calculated separately. Second, the compatibility equations associated with Eqs. (4) and (5) can be calculated independent of Eqs. (1), (2) and (3), however, again, the converse is not true. The full set of equations, Eqs. (1)-(5) must be used to calculate the compatibility equations for the gas phase.

With this information and the understanding that boundary conditions are strongly dependent on the characteristic equations, we shall make the assumption, that in determining the proper boundary conditions for our problem, we may treat the three gas equations and the two particle equations separately. The gas equations are then treated as completely hyperbolic, and possess the same boundary conditions as one-phase compressible flow. The one phase equations incorporating an ideal gas assumption will now be presented briefly. They are

$$\begin{aligned}\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} &= 0 \\ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} &= 0 \\ \frac{\partial}{\partial t} \left(\frac{p}{\rho \gamma} \right) + u \frac{\partial}{\partial x} \left(\frac{p}{\rho \gamma} \right) &= 0\end{aligned}$$

where

$$\frac{p}{p_0} = \left(\frac{c}{c_0} \right)^{2\gamma/(\gamma-1)}$$

The characteristic directions and their corresponding compatibility equations for this system are then

$$\begin{aligned}\text{along } \frac{dx}{dt} = u, & \quad d\left(\frac{p}{\rho \gamma} \right) = 0 \\ \text{along } \frac{dx}{dt} = u + c, & \quad du + \frac{c}{\gamma p} dp = 0 \\ \text{and along } \frac{dx}{dt} = u - c, & \quad du - \frac{c}{\gamma p} dp = 0\end{aligned}$$

For hyperbolic systems a properly posed set of initial and boundary conditions is relatively easy to determine. Courant and Friedrichs [18] discussed this problem in detail while introducing the concept of "space-like" and "time-like" curves. Essentially, they simply state

that for each characteristic reaching a point on a boundary from outside the domain, one dependent variable must be specified. As an example, let us take a typical boundary where the boundary coincides with a particle path, $dx/dt = u$. If this is a right boundary, the characteristic $dx/dt = u-c$ falls outside the region of interest, while if it is a left boundary the characteristic $dx/dt = u+c$ falls outside. In either case one dependent variable must be specified on each boundary.

In determining the proper initial conditions, we treat the initial time line as a boundary defined by $t=0$. For this case all three characteristics fall outside the domain and thus all three dependent variables, p , ρ and u must be specified.

For the problem presented in this report, we specify three gas properties on the initial time line and one gas property on each boundary as can be seen in the summary at the end of this section.

The determination of proper boundary conditions for the particle equations can not easily be placed on a rigorous foundation since they are parabolic in nature. It is felt, therefore, that insight into this problem could be gained by studying a few classical parabolic systems where proper boundary conditions have been established. Based on observation of these cases, we shall propose a hypothesis on boundary conditions, and apply it to our parabolic particle equations.

Boundary Condition Hypothesis

For two first order partial differential equations in terms of two dependent variables u and v , and two independent variables ξ and η ,

1. If $d\eta = 0$ is a degenerate characteristic, then there can be only one boundary at $\eta = \text{constant}$, along which either u or v may be prescribed. No boundary conditions need be prescribed on any other $\eta = \text{constant}$ line.
2. If one of the independent variables is time t , then only one boundary with $t = \text{constant}$ can exist, and further,
 - a. If $t = \text{constant}$ is a degenerated characteristic, either u or v may be specified;
 - b. If $t = \text{constant}$ is not a characteristic, both u and v must be specified, which is a typical Cauchy initial value problem.

Consider the system of equations

$$\frac{\partial v}{\partial \xi} = a \frac{\partial u}{\partial \eta} + \dots$$

$$\frac{\partial u}{\partial \xi} = v$$

(10)

which is equivalent to one second order equation

$$\frac{\partial^2 u}{\partial \xi^2} = a \frac{\partial u}{\partial \eta} + \dots$$

where the omitted terms do not contain any derivatives. For our present purpose, we shall use the first order system, instead of the single second order equation. It can be shown that for (10), $d\eta = 0$ is a characteristic line. According to our hypothesis, the boundary of the domain must be "open" in the positive η direction. Boundary condition can be specified along only one $\eta = \text{constant}$ line ([19], p. 692). If ξ is not the time coordinate, then two boundaries exist along two $\xi = \text{constant}$ lines

A typical problem of this nature is the heat transfer problem governed by the equation

$$\frac{\partial^2 T}{\partial x^2} = a^2 \frac{\partial T}{\partial t}$$

or the equivalent first order system

$$\frac{\partial G}{\partial x} = a^2 \frac{\partial T}{\partial t}$$

$$\frac{\partial T}{\partial x} = G$$

where T is temperature and a is a constant. The characteristic direction associated with this equation is

$$dt = 0.$$

A properly posed set of initial and boundary conditions for this problem, as shown in Fig. 2, is

$$\begin{aligned} t = 0 & \quad \text{specify } T \\ x = 0 & \quad \text{specify } T \\ x = L & \quad \text{specify } T \end{aligned}$$

where L is the thickness of the plate.

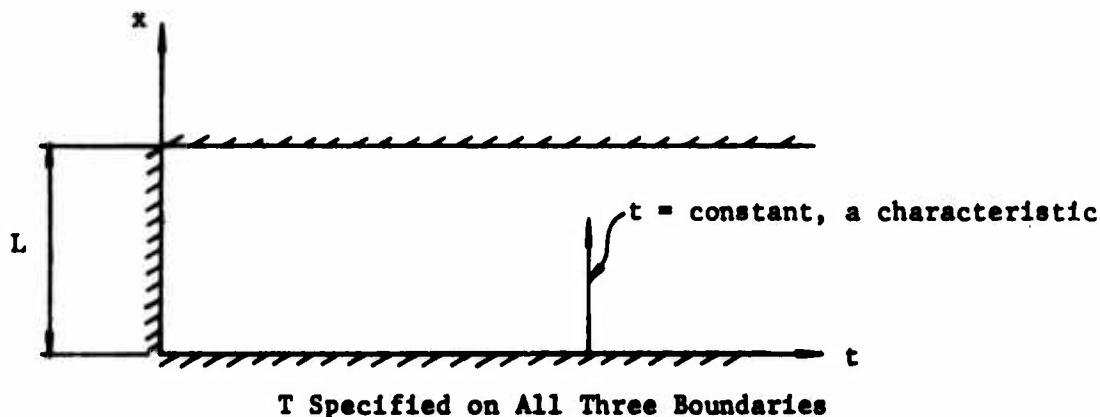


Figure 2 Boundary Conditions for the Heat Transfer Problem

Another example is the boundary layer equations. If only the terms relevant to our present discussion are included, the governing equation may be written as

$$\frac{\partial^2 u}{\partial y^2} = \frac{1}{\nu} u \frac{\partial u}{\partial x} + \dots$$

which has an equivalent first order system

$$\frac{\partial G}{\partial y} = \frac{1}{\nu} u \frac{\partial u}{\partial x} + \dots$$

$$\frac{\partial u}{\partial y} = G$$

where x is in the direction of flow and lies in the plane of the plate, y is normal to the plane of the plate, u is the velocity in the x direction and ν is the kinematic viscosity. The characteristic direction for this system is

$$dx = 0$$

A properly posed set of boundary conditions for this problem as shown in Fig. 3 is

$$\begin{aligned} y = 0 & \quad \text{specify } u \\ y \rightarrow \infty & \quad \text{specify } u \\ x = x_0 & \quad \text{specify } u(x_0, y) \end{aligned}$$

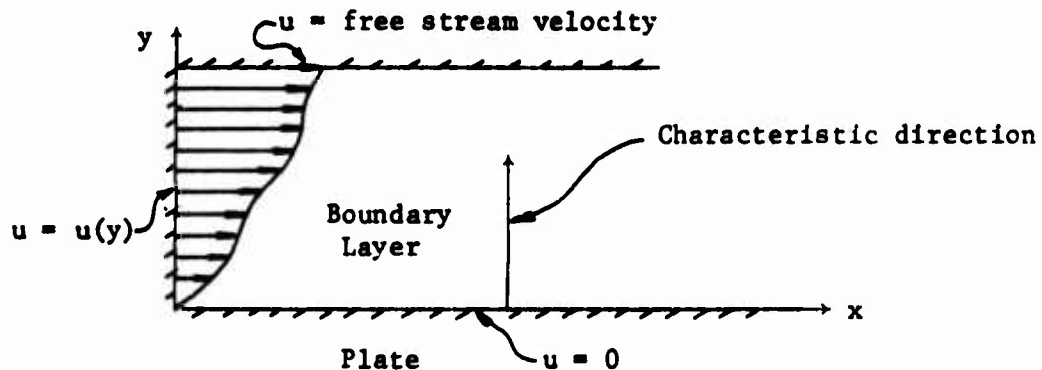


Figure 3 Boundary Conditions for Boundary Layer Flow

In both of these examples, ξ is not the time coordinate. In our particle phase case, the equations may be represented by

$$\frac{D^p \sigma_p}{Dt} = -\sigma_p \frac{\partial u}{\partial x} + \dots$$

$$\frac{D^p u_p}{Dt} = \dots$$

where the independent variable equivalent of ξ of Eq. (10) is time. Therefore, only one $\xi = \text{constant}$ boundary exists, as shown in Fig. 4.

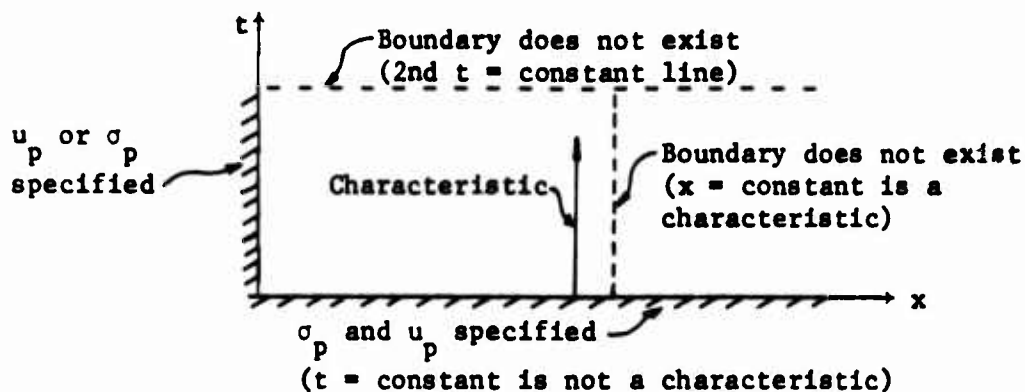


Figure 4 Boundary Conditions for the Particle Phase of Our Flow

In the actual problem, the right hand side of the domain is bounded by a gas-particle interface, see Fig. 5. No boundary conditions need be specified on this boundary for the particles, the solution of the gas equations and the particle equations will yield the location of this interface line.

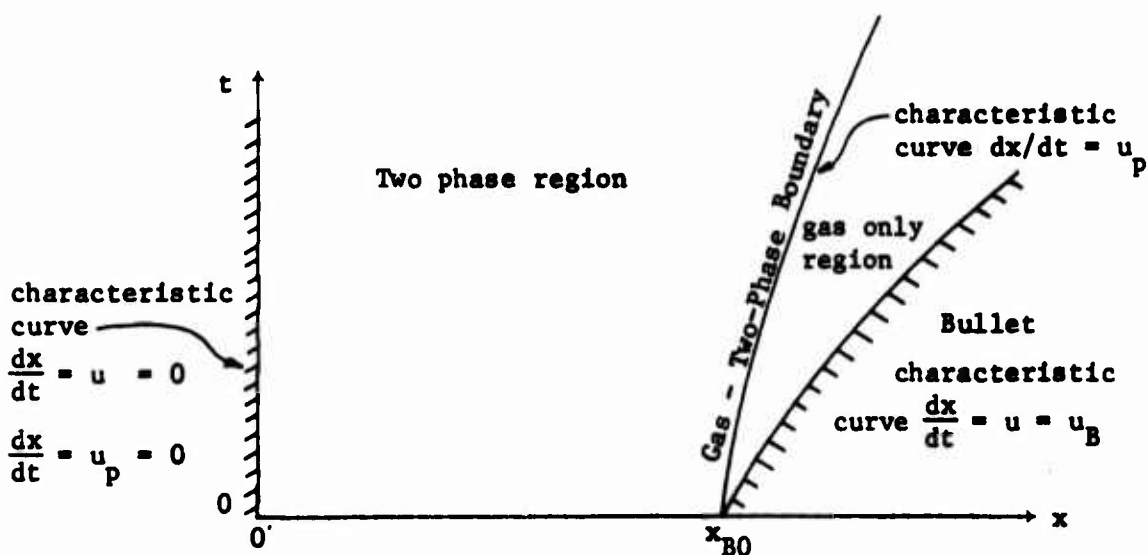


Figure 5 Physical Plane Description of Two Phase Flow Behind a Projectile

In summary, the boundary conditions for our problem are Breech ($x=0$)

$$u(0,t) = 0$$

$$u_p(0,t) = 0$$

Left Bullet surface ($x = x_B$) and ($x < x_M$)

$$u_B = \frac{dx_B}{dt}$$

$$\frac{du_B}{dt} = - \frac{1}{M_B} [F_R - (p_{BEF} - p_{AFT})A_B]$$

$$u(x_B, t) = u_B$$

Right Bullet surface ($x = x_B + L_B$)

$$u(x_B + L_B, t) = u(x_B, t)$$

Muzzle - after bullet has left ($x = x_M$)

$$p(x_M, t) = p_{BEX} + (p_M - p_{BEX})(t - t_{EX})/t_{BD}$$

$$\text{when } [u(x_M, t) < c(x_M, t)]$$

or

$$u(x_M, t) = c(x_M, t)$$

Muzzle - before bullet has left ($x = x_M$)

$$p(x_M, t) = p_M \quad \text{when } [u(x_M, t) < c(x_M, t)]$$

or

$$u(x_M, t) = c(x_M, t)$$

Muzzle - after shock has left ($x=x_M$)

$$p(x_M, t) = p_{EXIT} + (p_M - p_{EXIT})(t - t_{EXIT})/t_{SD}$$

$$\text{when } [u(x_M, t) < c(x_M, t)]$$

or

$$u(x_M, t) = c(x_M, t)$$

Initial time line ($t=0$)

$$u(x, 0) = f_1(x)$$

$$p(x, 0) = f_2(x)$$

$$\rho(x, 0) = f_3(x)$$

$$e(x, 0) = f_4(x)$$

$$u_p(x, 0) = f_5(x)$$

$$\rho_p(x, 0) = \text{constant}$$

5. Shock Waves

The treatment of shock waves presented here is based on the hypothesis that when a shock wave passes through a particle-laden gas, the changes occur at such a rapid rate that immediately behind the wave the particles have not had sufficient time to react. The shock wave produces a rapid deceleration of the gas accompanied by a nearly discontinuous rise in pressure. Therefore, as presented by Kriebel [21] and Rudinger [10], the initial disturbance caused by the shock wave is not influenced by the presence of particles in the gas. All properties behind the shock can be calculated from the shock conditions if the gas properties in front of the wave are known along with the shock speed or one gas property behind the wave. This state immediately behind the wave is known as the "frozen" state.

The equations used to calculate the gas properties in the frozen state are the standard Rankine-Hugoniot shock relations

$$\rho_1 (U-u_1) = \rho_2 (U-u_2) \quad (11)$$

$$p_2 - p_1 = \rho_1 (U-u_1)(u_2-u_1) \quad (12)$$

$$E_2 - E_1 = \frac{1}{2} (p_2 - p_1) \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right) \quad (13)$$

where subscripts 1 and 2 represent properties in front of and behind the shock, respectively, and U is the shock speed. As previously mentioned, the properties of the particles are identical in front of and behind the wave.

6. Equation of State

In formulating the governing equations, it was only natural to assume that the equation of state was a function of the specific internal energy, E , and the density, ρ or

$$p = p(\rho, E) \quad (14)$$

However, in the practical application of flow in a gun barrel, the equation of state will more than likely be given in the form

$$p = p'(\rho, T) \quad (15)$$

therefore, provision must be made to incorporate this form into our formulation. In this section we will treat the subject in detail and present specific examples.

From the mathematical standpoint, if we can arrive at a relation between E , T , and ρ of the form

$$f(E, T, \rho) = 0 \quad (16)$$

then Eqs. (15) and (16) will combine to be equivalent to Eq. (14).

The procedure used to generate Eq. (16) involves the solution of several partial differential equations from classical thermodynamics [22]. In order to solve these equations two conditions must be specified. First, $C_v(\rho_0, T)$ must be given, which for this problem it is assumed to be of the form

$$C_v(\rho_0, T) = A_1 + A_2 T$$

Secondly, the constant $E(\rho_0, T_0)$ must be given. Knowing these two conditions, we can proceed to determine Eq. (16).

We begin by calculating the constant volume specific heat of the gas by solving the equation

$$\frac{\partial C_v}{\partial \rho} = - \frac{1}{\rho^2} T \frac{\partial^2 p'}{\partial T^2}$$

Then, we calculate $E(\rho, T)$ and subsequently Eq. (16) from the relations

$$\frac{\partial E}{\partial T} = C_v$$

and

$$\frac{\partial E}{\partial \rho} = - \frac{1}{\rho^2} (T \frac{\partial p'}{\partial T} - p')$$

and the condition $E(\rho_0, T_0)$.

Determining Eq. (16) only conceptually solves the problem of handling an equation of state in the form of Eq. (15). At this point we will treat the actual technique for implementing Eqs. (15) and (16) into the computer code.

When the value of p must be calculated, assuming that ρ and E are known, Eq. (16) is solved numerically for T and then T and ρ are substituted into Eq. (15) to yield p . When the derivatives $\frac{\partial p}{\partial \rho}$ and $\frac{\partial p}{\partial E}$ are required, they are calculated from Eqs. (15) and (16) through the following formulas

$$\frac{\partial p}{\partial E} = \frac{\partial p'}{\partial T} \frac{\partial T(\rho, E)}{\partial E}$$

$$\frac{\partial p}{\partial \rho} = \frac{\partial p'}{\partial T} \frac{\partial T(\rho, E)}{\partial \rho} + \frac{\partial p'}{\partial \rho}$$

Where the value of $\frac{\partial T}{\partial E}$ and $\frac{\partial T}{\partial \rho}$ are found from Eq. (16) using the relations

$$\frac{\partial T}{\partial E} = - \frac{\frac{\partial f}{\partial E}}{\frac{\partial f}{\partial T}}$$

and

$$\frac{\partial T}{\partial \rho} = - \frac{\frac{\partial f}{\partial \rho}}{\frac{\partial f}{\partial T}}$$

We will now present two equations of state which have been implemented into the computer code. The first is the "virial equation" given by

$$p = \rho \frac{R}{M} T [1 + \rho B(T) + \rho^2 C(T)] \quad (17)$$

and the second is the van der Waals equation given by

$$p = \rho \frac{R}{M} T \left(\frac{1}{1 - \eta \rho} \right) - \alpha \rho^2 \quad (18)$$

where R/M , η , and α are constants which are material dependent and $B(T)$ and $C(T)$ are empirically determined functions of temperature. It should be noted that if α is set equal to zero Eq. (18) is the Noble-Abel equation of state and if both α and η are set equal to zero it becomes the ideal gas equation of state.

The values of C_v and $f(\rho, E, T)$ corresponding to Eq. (17) are given by

$$C_v(\rho, T) = A_1 + A_2 T - (\rho - \rho_0) \frac{RT}{M} \frac{\partial^2}{\partial T^2} \{ T [B(T) + \frac{1}{2} (\rho + \rho_0) C(T)] \}$$

$$f(\rho, E, T) = E - E(\rho_0, T_0) - A_1(T - T_0) - \frac{1}{2} A_2(T^2 - T_0^2) + \frac{RT^2}{M} (\rho - \rho_0) \left[\frac{\partial B(T)}{\partial T} + \frac{1}{2} (\rho + \rho_0) \frac{\partial C(T)}{\partial T} \right] = 0$$

while the values corresponding to Eq. (18) are given by

$$C_v(\rho, T) = C_{v0}(\rho_0, T) = A_1 + A_2 T$$

$$f(\rho, E, T) = E - E(T_0, \rho_0) - A_1(T - T_0) - \frac{1}{2} A_2(T^2 - T_0^2) + \alpha(\rho - \rho_0) = 0$$

As additional equations of state become available they may easily be incorporated into the code.

7. Area Discontinuity (gas-particle interface)

In order to examine the behavior of a two-phase material as it passes through an area discontinuity, moving at a velocity u_D , let us construct a control volume as shown in Fig. 6. (it should be noted that for the gas particle interface $u_D = u_p$). It is convenient to treat section B as an exit from the "main" flow field and section A as an entrance back

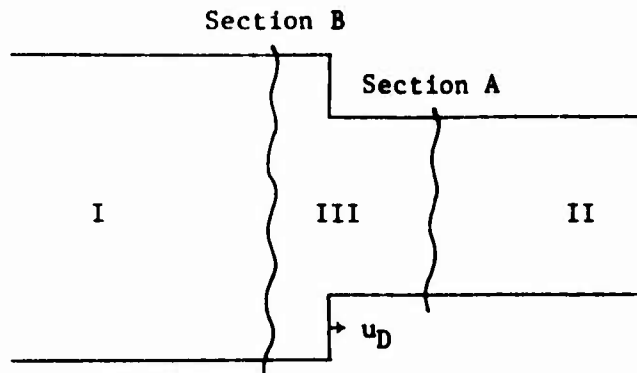
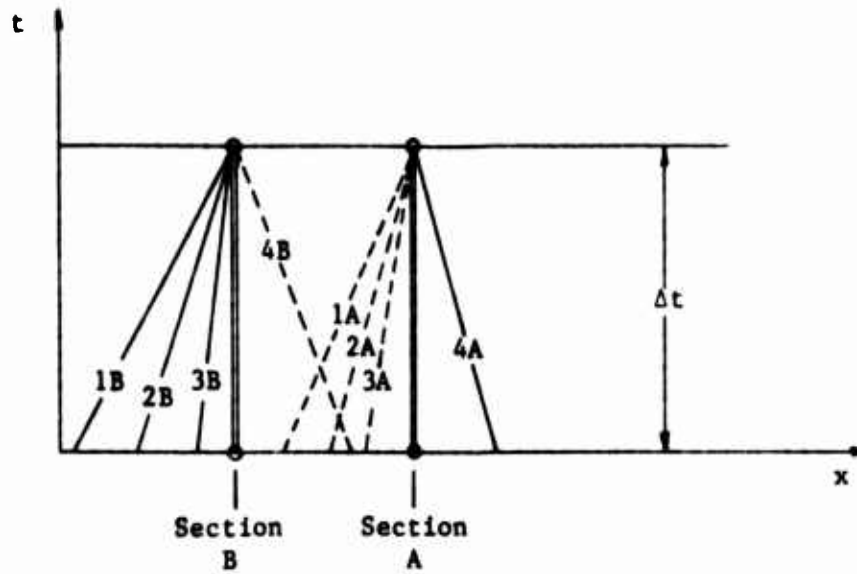


Figure 6. Area Discontinuity

into the field. Thus section A may be considered as the entrance of region II, and section B as the exit from region I. These two regions are coupled by constraints relating their respective properties across the control volume, region III. In the limit, we may let region III shrink to a line located at the area discontinuity. We will now determine these constraints. First we note in Fig. 7 that four of the characteristic lines fall outside the main flow field: namely characteristics 4B, at section B, and 1A, 2A and 3A at section A. Equations written along these lines must therefore be replaced. In Sec. (III,1) it is shown that one compatibility equation is associated with each of the four above-mentioned characteristic directions; in addition, the particle continuity equation is written in finite-difference form along the characteristic 3A ($\frac{dx}{dt} = u_p$). Thus there are five missing equations which must be replaced by five new relations coupling the properties of section A with those of section B.

Let us now determine these new equations. Since the particle equations are weakly coupled to the gas equations, the characteristic directions can be associated distinctly with either the gas or the particle phase. We shall assume that the equations written along "gas" characteristics ($\frac{dx}{dt} = u \pm c$, u) should be replaced by equations relating gas properties, and that equations written along the "particle" characteristic ($\frac{dx}{dt} = u_p$) should be replaced by equations relating particle properties. Therefore we will need three equations governing the



$$(1B) \quad \frac{dx}{dt} = u_B + c_B$$

$$(1A) \quad \frac{dx}{dt} = u_A + c_A$$

$$(2B) \quad \frac{dx}{dt} = u_B$$

$$(2A) \quad \frac{dx}{dt} = u_A$$

$$(3B) \quad \frac{dx}{dt} = u_{pB}$$

$$(3A) \quad \frac{dx}{dt} = u_{pA}$$

$$(4B) \quad \frac{dx}{dt} = u_B - c_B$$

$$(4A) \quad \frac{dx}{dt} = u_A - c_A$$

Figure 7. Physical plane (x,t) plot of area discontinuity showing characteristic network.

change in gas properties between sections A and B, and two equations relating particle properties.

First, let us consider the relations for the gas phase. Our treatment essentially follows that given by Shapiro [23]. In his approach, mass and energy are conserved between the two sections; momentum conservation is not considered, because to do so would require knowledge of the forces acting between the wall and the fluid. In place of momentum conservation, Shapiro makes the simplifying assumption that entropy is continuous across the area change. For our problem, it seems that this assumption is satisfactory. However, if entropy calculations are prohibitively difficult because of the complexity of the particular equation of state chosen, then either the assumption of constant temperature between the sections or the momentum equation utilizing an approximation for the pressure on the wall may be used.

Let us now determine the two equations governing the change in particle properties*. One relation which is easily obtained is conservation of mass between the sections, namely:

$$\sigma_{pA}(u_{pA} - u_D)A = \sigma_{pB}(u_{pB} - u_D)A_B$$

The remaining equation is more difficult to determine. As was the case for the gas phase, applying the principle of conservation of momentum would require knowledge of the interaction force between the wall and the particles; thus rendering its use impractical. The equation of energy conservation for the particle phase, although it could be applied, would not complete the system of equations since it is uncoupled from the system, and thus would merely add one equation and one new variable E_p . Entropy calculations are impossible for the model ignores the thermodynamic aspects of the particle phase.

One possible approach is to assume that the particle velocity does not vary across the area discontinuity. This supposition is reasonable when one considers that, although the gas phase velocity increases instantaneously, the particles, being more massive, do not accelerate as quickly. (Such an approximation brings to mind the assumption of frozen flow used to calculate property changes across shock waves; see section II(5).) For area discontinuities, this approximation seems valid if ϵ is small or if the area change is from small to large; however, inconsistencies (such as $\epsilon > 1$) may arise with flows in which a highly concentrated particle phase travels from a large area to a smaller one. For this reason, we have chosen to write the last of the five equations in the form:

$$(u_p)_A = K_m (u_p)_B$$

where K_m is a factor which, most likely, depends on geometry and flow parameters and must be determined experimentally.

* Note that for the gas-particle interface these equations are not necessary since particles do not exist at Section B.

For the present, we have made the convenient assumption that

$$\epsilon_A = \epsilon_B,$$

which when combined with the mass conservation equation yields

$$K_m = \frac{A_B}{A_A}$$

It is yet to be seen how the factor K_m affects the overall flow calculations. To summarize, the equations which will be used are, for the gas phase,

Conservation of mass

$$\sigma_A(u_A - u_D)A_A = \sigma_B(u_B - u_D)A_B \quad (19)$$

Conservation of energy

$$(H + \frac{u^2}{2})_A = (H + \frac{u^2}{2})_B \quad (20)$$

Continuity of entropy

$$S_A = S_B \quad (21)$$

and for the particle phase,

Conservation of mass

$$\sigma_A(u_{pA} - u_D)A_A = \sigma_B(u_{pB} - u_D)A_B \quad (22)$$

Particle velocity assumption

$$(u_p)_A = K_m (u_p)_B \quad (23)$$

8. Mass Transfer Between Solid and Gas Phase

Following the procedure used to calculate the rate at which heat is released while the propellant is burning we define the mass of an individual particle, M_p , as

$$M_p = V_p \sigma_p$$

The rate at which the mass of a single particle is changing due to burning, \dot{M}_p , is then given by

$$\dot{M}_p = \frac{D^P}{Dt} M_p = \rho_p \frac{D^P V_p}{Dt}$$

where

$$\frac{D^P V_p}{Dt} = \frac{1}{S_p(z)} \frac{D^P z}{Dt}$$

and $S_p(z)$ is the burning surface

Defining the number of particles per unit volume of mixture, N , as

$$N = \frac{1}{V_p} \frac{\sigma_p}{\rho_p} = \frac{\epsilon}{V_p}$$

we then can define the rate at which mass is being added to the gas phase per unit volume of mixture, ω , as

$$\omega = - \dot{M}_p N = - \frac{\epsilon}{V_p} \frac{D^p V_p}{Dt} \quad (24)$$

9. Burning Law (Regression Equation)

Before introducing the specific equation specifying the regression rate, let us first define the regression distance $Z(x,t)$. To do this we define a parameter ψ to be a characteristic dimension of a propellant grain in the sense that it is the least dimension which has to be traveled by the burning surface in order to burn the propellant completely. The regression distance is then defined as the amount that ψ has decreased from its initial value at a particular x and t . The regression rate is then simply DPZ/DT . The specific form currently being used is the non-linear burning law given by

$$\frac{DPZ}{Dt} = \alpha(T) p^\beta \quad (25)$$

10. Heat Released During the Burning of the Propellant

In order to calculate q , the amount of heat released during a given time interval, we must be able to calculate the volume of the propellant burnt at any instant, $V_b(x,t)$; or equivalently, the instantaneous particle volume $V_p(x,t)$ recognizing that the two are related we can write

$$\frac{DPV_b(x,t)}{Dt} = - \frac{DPV_p}{Dt} \quad (26)$$

If we now define a parameter K_Q as the amount of heat released per unit volume of propellant burnt, then the rate at which an individual particle is giving off heat is thus given by

$$\frac{DPQ_p}{Dt} = K_Q \frac{DPV_b}{Dt} = - K_Q \frac{DPV_p}{Dt} \quad (27)$$

Now defining N_g , the number of particles per unit mass of gas as

$$N_g = \frac{\sigma_p}{\sigma V_p \rho_p} = \frac{\epsilon}{\sigma V_p} \quad (28)$$

we can calculate, q , the rate at which heat is being added to the gas phase per unit mass of gas by

$$q = N_g \frac{D^P Q^*}{Dt} \quad (29)$$

Equation (29) can be combined with Eqs. (24), (27) and (28) to yield

$$q = - N_g K_Q \frac{D^P v_p}{Dt} = \frac{\omega}{\rho_p \sigma} K_Q \quad (30)$$

11. Calculation of the Initiation and Tracing of a Shock Wave Behind the Bullet

Here we present techniques used to insert and trace a shock wave behind the bullet. These procedures will handle shock reflection from both the breach and the bullet precisely; however, some order of approximation will be necessary to treat a shock passing through a gas-particle interface.

It is proposed to calculate the singularity occurring at this interaction point precisely and then "smear" the reflected wave to simplify future calculations. The wave structure of this interaction point is shown in Figs. (8) and (9). Figure (8) shows the interaction of a right-traveling shock with the gas-particle interface. The procedure for calculating this singularity is:

- a. Calculate the properties in regions a,b and c and assign them to the mesh points as shown.
- b. Calculate the properties in regions 2,3 and 5 (region 4 notation is not used due to programming considerations) ($a \leftrightarrow 1$ and $c \leftrightarrow 6$)
- c. Assign the properties in regions 2,3,5 and 6 to mesh points as shown. This has the effect of causing the properties, starting at point I, to vary gradually until they reach the values of region 2 just before the gas particle interface. A precise treatment would cause the properties in region 1 to be gradually reached at the gas particle interface and then change instantaneously to those in region 2, see Fig. (10). (The properties in region 1 are not retained for future calculation).

It should also be noted that the contact surface is not traced in subsequent calculations.

Figure (9) shows the interaction of a left traveling shock with the gas-particle interface. The calculation procedure here is quite similar to that used for a right traveling wave and is as follows:

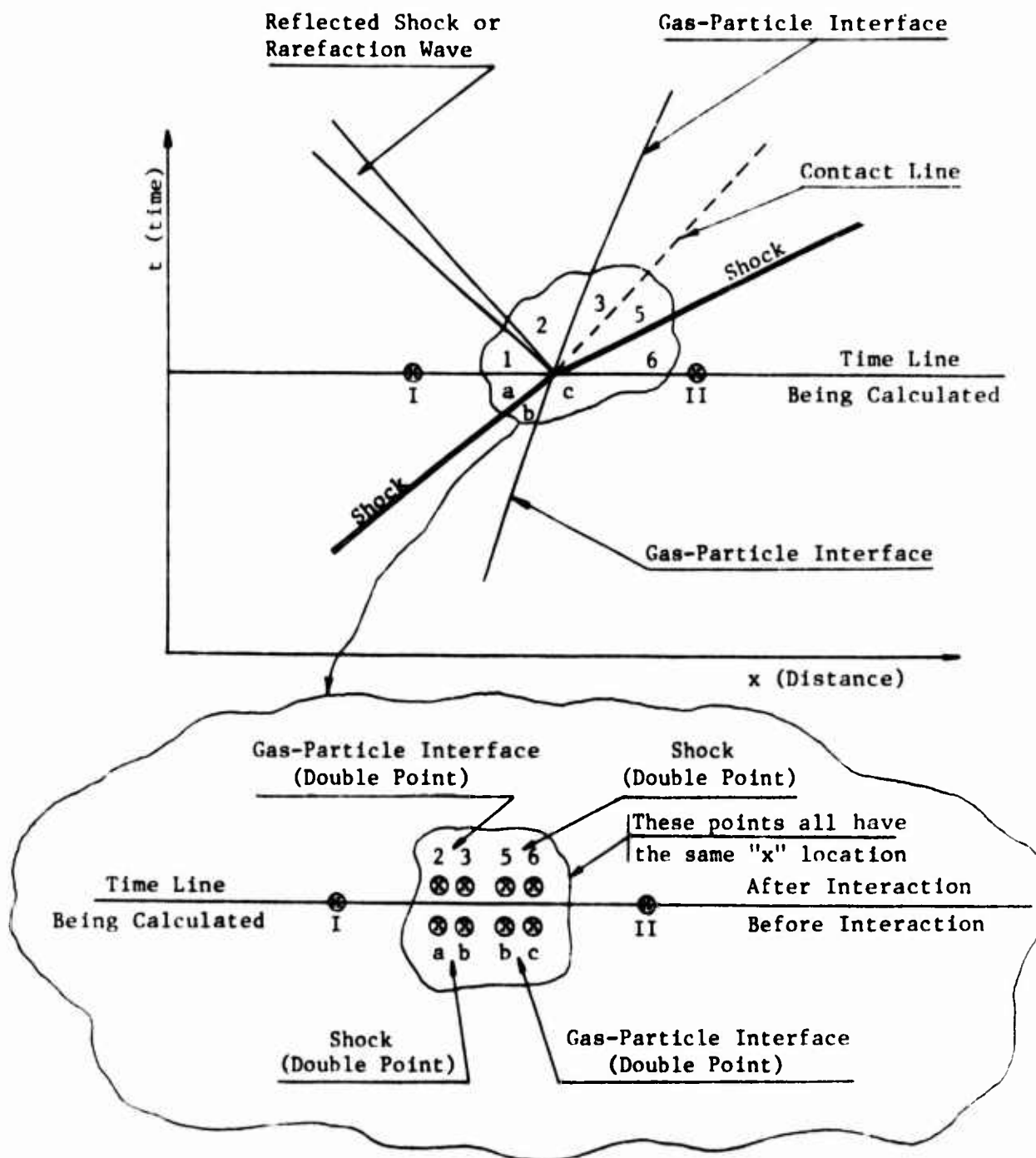


Figure 8. A Right Traveling Shock Wave Interacting With a Gas-Particle Interface.

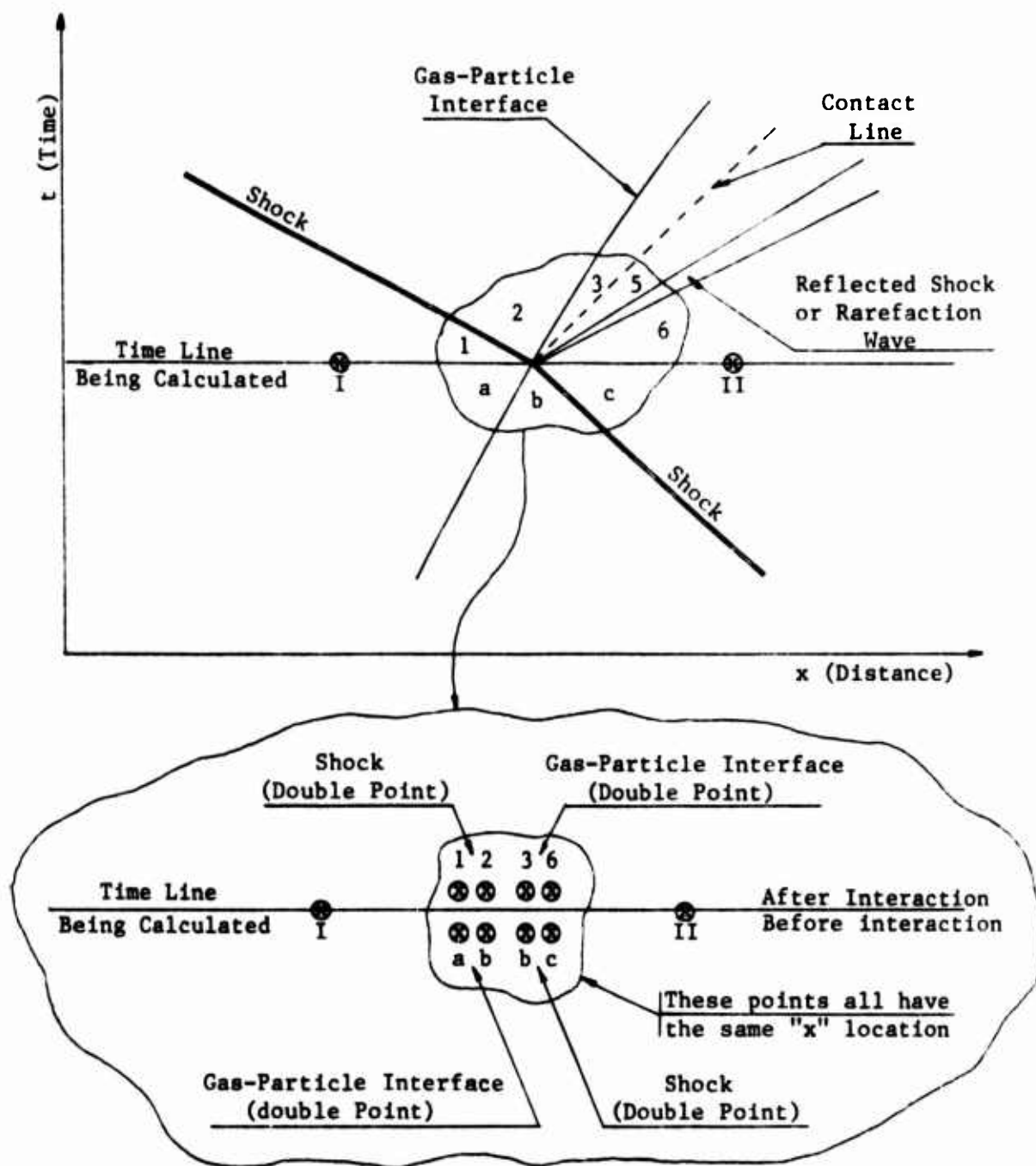


Figure 9. A Left Traveling Shock Wave Interacting With a Gas-Particle Interface.

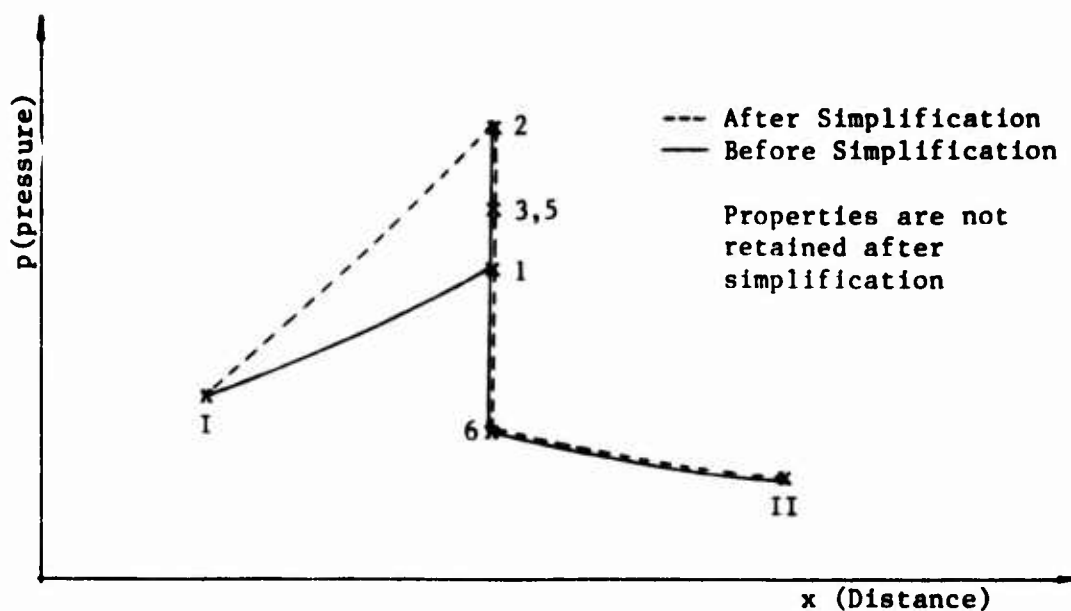


Figure 10. Pressure vs Position Plot Showing Singularity Properties Before and After Simplification for a Right Traveling Shock Intersecting with a Gas-Particle Interface.

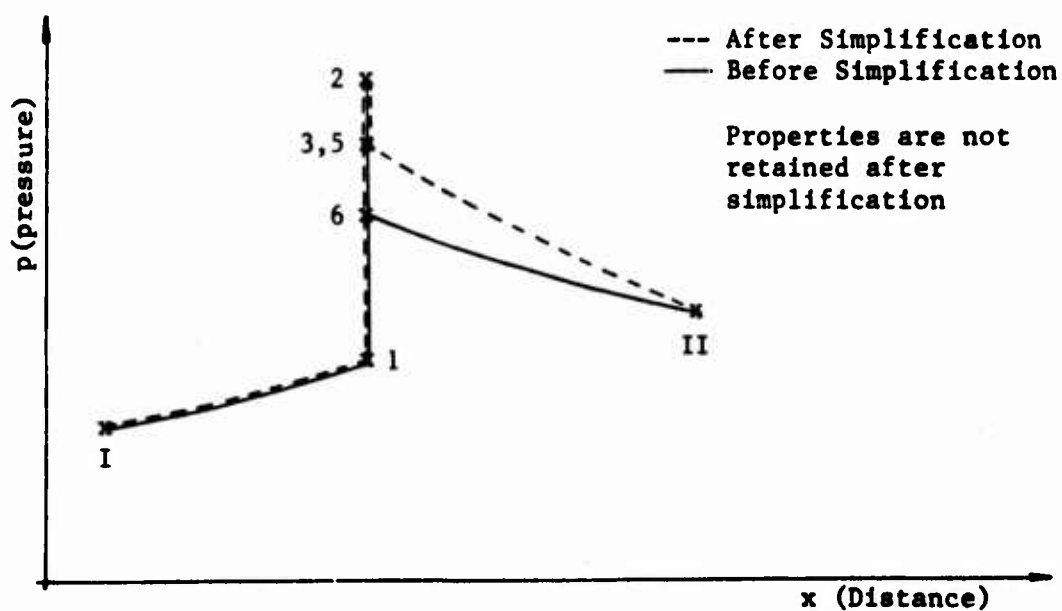


Figure 11. Pressure vs Position Plot Showing Singularity Properties Before and After Simplification for a Left Traveling Shock Intersecting with a Gas-Particle Interface.

- a. Calculate the properties in regions a,b and c and assign them to the mesh points as shown.
- b. Calculate the properties in regions 2,3 and 5 (region 4 notation is not used due to programming considerations). (a \leftrightarrow 1 and c \leftrightarrow 6)
- c. Assign the properties in regions 1,2,3 and 6 to mesh points as shown. This has the effect of causing the properties, starting at point II, to vary gradually until they reach the values of region 3 just after the interface. A precise treatment would cause the properties in region 6 to be reached just after the interface and then change instantaneously in two steps to those in regions 5 and 3, see Fig. (11). (The properties in regions 5 and 6 are not retained for future calculations)

It should be noted that the contact surface is not traced in subsequent calculations.

The simplifications that we use in treating the shock-interface singularity and in the subsequent calculations seem to produce errors which are, for the most part, dependent on the mesh size (the smaller the mesh, the more accurate the smoothing) and the magnitude of ϵ (the smaller the value of ϵ , the smaller the reflected wave). One will have to judge on an individual-problem basis the magnitude of these errors.

III. NUMERICAL PROCEDURE (THE METHOD OF CHARACTERISTICS)

1. Calculation of the Characteristic Directions and Compatibility Equations

Before calculating the compatibility equations corresponding to Eqs. (1) to (11) let us eliminate the partial derivatives of p and ϵ from Eqs. (2), (3) and (6) by using Eqs. (7), (8) and (9). We then arrive at the partial differential equations that are used in the computer code, namely:

gas continuity

$$\sigma_{,t} + u \sigma_{,x} + \sigma u_{,x} = GC \quad (31)$$

gas momentum

$$u_{,t} + u u_{,x} + A \sigma_{,x} + B E_{,x} + D \sigma_{p,x} = GM \quad (32)$$

gas energy

$$E_{,t} + u E_{,x} + F u_{,x} + G \sigma_{p,x} = GE \quad (33)$$

particle continuity

$$\sigma_{p,t} + u_p \sigma_{p,x} + \sigma_p u_{p,x} = PC \quad (34)$$

particle momentum

$$u_{p,t} + u_p u_{p,x} = PM \quad (35)$$

and particle energy

$$E_{p,t} + u_p E_{p,x} + H u_{p,x} + J \sigma_{p,x} = PE \quad (36)$$

where

$$A = \frac{1}{\sigma} p_{,\rho} ; \quad B = \frac{(1-\epsilon)}{\sigma} p_{,E} ;$$

$$D = \frac{1}{\rho_p (1-\epsilon)} p_{,\rho} ; \quad F = \frac{p}{\rho} ;$$

$$G = \frac{p u}{\rho_p \sigma} ; \quad H = \frac{p}{\rho_p}$$

$$J = \frac{p u_p}{\rho_p \sigma_p}$$

GC , GM , GE , PC , PM , and PE are the right hand side of Eqs. (1) to (11), respectively and the notation $X_{,y}$ represents the partial derivative of X with respect to y .

The characteristic directions and compatibility equations for this system of equations has been calculated using both the directional derivative approach and the determinant approach producing identical results. Only the determinant approach will be presented here.

In applying the determinant approach, we treat the time and spatial derivatives of the dependent variables as unknown quantities. If we add the six continuity equations

$$d\sigma = \sigma_{,x} dx + \sigma_{,t} dt \quad (37)$$

$$du = u_{,x} dx + u_{,t} dt \quad (38)$$

$$dE = E_{,x} dx + E_{,t} dt \quad (39)$$

$$d\sigma_p = \sigma_{p,x} dx + \sigma_{p,t} dt \quad (40)$$

$$du_p = u_{p,x} dx + u_{p,t} dt \quad (41)$$

$$dE_p = E_{p,x} dx + E_{p,t} dt \quad (42)$$

to our system of partial differential equations we arrive at a system of 12 equations in terms of 12 derivatives which when written in matrix notation becomes:

$$\begin{bmatrix} u & 1 & \sigma & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ A & 0 & u & 1 & B & 0 & D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & F & 0 & u & 1 & G & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & u_p & 1 & \sigma_p & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & u_p & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & H & 0 & u_p & 1 \\ dx & dt & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & dx & dt & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & dx & dt & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & dx & dt & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & dx & dt & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & dx & dt \end{bmatrix} \begin{bmatrix} \sigma_{,x} \\ \sigma_{,t} \\ u_{,x} \\ u_{,t} \\ E_{,x} \\ E_{,t} \\ \sigma_{p,x} \\ \sigma_{p,t} \\ u_{p,x} \\ u_{p,t} \\ E_{p,x} \\ E_{p,t} \end{bmatrix} = \begin{bmatrix} GC \\ GM \\ GE \\ PC \\ PM \\ PE \\ d\sigma \\ du \\ dE \\ d\sigma_p \\ du_p \\ dE_p \end{bmatrix} \quad (43)$$

Let N^* be the determinant of the coefficient matrix appearing in Eq. (43) and M_i be the determinant of the matrix formed from the coefficient matrix with the i^{th} column replaced by the column vector on the right hand side of Eq. (43). The solution for the derivatives may then be written in the form

$$N^* \sigma_{,x} = M_1 ; N^* \sigma_{,t} = M_2 ; \text{ etc.} \quad (44)$$

The characteristic directions for this system of equations are defined as directions in the x, t -plane which cause

$$N^* = 0.$$

In solving for these directions, it is convenient to reduce the 12×12 determinant N^* through column operations and Laplace expansion [24], to the following form,

$$N^* = \begin{vmatrix} dx-udt & -\sigma dt & 0 & 0 & 0 & 0 \\ -A dt & dx-udt & -B dt & -D dt & 0 & 0 \\ 0 & -F dt & dx-udt & -G dt & 0 & 0 \\ 0 & 0 & 0 & dx-u_p dt & -\sigma_p dt & 0 \\ 0 & 0 & 0 & 0 & dx-u_p dt & 0 \\ 0 & 0 & 0 & -J dt & -H dt & dx-u_p dt \end{vmatrix} \quad (45)$$

$$= \begin{vmatrix} dx-udt & -\sigma dt & 0 \\ -A dt & dx-udt & -B dt \\ 0 & -F dt & dx-udt \end{vmatrix} \times \begin{vmatrix} dx-u_p dt & -\sigma dt & 0 \\ 0 & dx-u_p dt & 0 \\ -J dt & -H dt & dx-u_p dt \end{vmatrix}$$

or

$$N^* = (dx - udt)[dx - (u + c)dt][dx - (u - c)dt](dx - u_p dt)^3 = 0$$

where

$$c^2 = \sigma A + (B)(F) = \frac{\partial p}{\partial \rho} + \frac{p}{2} \frac{\partial p}{\partial E}$$

Thus the characteristic directions are

$$\frac{dx}{dt} = u ; \quad \frac{dx}{dt} = u + c ; \quad \frac{dx}{dt} = u - c$$

and

$$\frac{dx}{dt} = u_p \quad (46)$$

where $\frac{dx}{dt} = u_p$ is a triple degenerate root.

It can be seen that in order to have a finite solution for the partial derivatives in Eq. (44), the M_1 must equal zero when N equals zero. The setting of the M_1 determinants equal to zero leads either to an identity, zero equals zero, or to one compatibility equation corresponding to each of the characteristic directions (note that it is possible for as many as three distinct compatibility equations to exist along the triple degenerate root $\frac{dx}{dt} = u_p$). For this system, only one distinct compatibility equation exists along $\frac{dx}{dt} = u_p$, which indicates that the system is not totally hyperbolic and thus other equations in addition to the compatibility equations are needed to complete the solution.

The compatibility equations for this system are

$$\begin{aligned} \text{along } \frac{dx}{dt} = u \\ G[\sigma_p du_p - (u_p - u)d\sigma_p] + (u_p - u)^2 (dE - \frac{F}{\sigma} d\sigma) \\ = \{G[\sigma_p PM - (u_p - u) PC] + (u_p - u)^2 [GE - \frac{F}{\sigma} GC]\}dt \end{aligned} \quad (47)$$

$$\begin{aligned} \text{along } \frac{dx}{dt} = u \pm c \\ (G \times B \pm D \times c) [\sigma_p du_p - (u_p - u \mp c) d\sigma_p] \\ + (u_p - u \mp c)^2 [B dE \pm c du + A d\sigma] = \\ (G \times B \pm D \times c) [\sigma_p PM - (u_p - u \mp c) PC] \\ + (u_p - u \mp c)^2 [B \times GE \pm c \times GM + A GC] \}dt \end{aligned} \quad \begin{aligned} (48) \\ (49) \end{aligned}$$

$$\text{and along } \frac{dx}{dt} = u_p$$

$$du_p = PM dt \quad (50)$$

As mentioned before, there are two compatibility equations missing. Thus, two additional equations must be supplied. We will follow a procedure similar to that used in Refs. [6] and [9] for one-dimensional two-phase flow and Refs. [25] and [26] for two-dimensional flows and write Eqs. (34) and (36) in finite difference form along the particle path line of the particle phase ($dx/dt = u_p$) namely:

$$\frac{D^P \sigma}{Dt} + \sigma_p u_{p,x} = PC \quad (51)$$

and

$$\frac{D^P E}{Dt} + H u_{p,x} + J \sigma_{p,x} = PE \quad (52)$$

The addition of Eqs. (51) and (52) to our numerical procedure necessitates the calculation of $u_{p,x}$ and $\sigma_{p,x}$ at the new point.

To accomplish this we follow a procedure similar to that used in Ref. [6] and write the "continuity" equation for u_p and σ_p along the gas characteristics, $dx/dt = u \pm c$, namely:

$$d u_p = [u_{p,x} (u \pm c) + u_{p,t}] dt \quad (53)$$

and

$$d \sigma_p = [\sigma_{p,x} (u \pm c) + \sigma_{p,t}] dt \quad (54)$$

Equations (47) to (54), after being written in a second order accurate finite-difference form, will be used to generate a solution to the problem.

Our general numerical procedure will utilize the Hartree (constant time) scheme. In this scheme, it is assumed that the values of all dependent variables are known at discrete mesh points lying on a constant time line. A new time line is established to meet a stability criterion and the properties are calculated at points where the gas particle path originating from the known points on the old time line intersects the new time line.

The only problem that arises in the use of this technique concerns Eqs. (53) and (54). As can be seen, the time and spacial derivatives of u_p and σ_p must be available on the old time line before the new time plane can be calculated. If the values of u_p and σ_p and not their derivatives are specified on an initial constant time line the x derivatives will be calculated using 3 point forward or backward difference schemes for the left and right boundaries respectively and central difference for interior points and then Eqs. (4) and (5) will be solved for the time derivatives. These values will then be stored for use in calculating the next time line.

2. Mathematical Implications of the Physical Assumptions

Before examining the effects that our physical assumptions have on the characteristics, let us see what we can conclude in general about our system of equations. To do this let us partition the determinant N^* , Eq. (45), into 4 minors, namely

$$N^* = \begin{vmatrix} Q_1 & Q_2 \\ - & - \\ Q_3 & Q_4 \end{vmatrix}$$

where

$$Q_1 = \begin{vmatrix} dx-udt & -\sigma dt & 0 \\ -A dt & dx-udt & -B dt \\ 0 & -F dt & dx-udt \end{vmatrix}$$

$$Q_2 = \begin{vmatrix} 0 & 0 & 0 \\ -D dt & 0 & 0 \\ -G dt & 0 & 0 \end{vmatrix}$$

$$Q_3 = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix}$$

$$Q_4 = \begin{vmatrix} dx-u_p dt & -\sigma dt & 0 \\ 0 & dx-u_p dt & 0 \\ -J dt & -H dt & dx-u_p dt \end{vmatrix}$$

Applying Laplace expansion to N we can see that if all the terms in Q_3 are zero (the particle equations are weakly coupled to the system, [24]),

$$N^* = |Q_1| \times |Q_4|.$$

Thus, as long as $Q_3 = 0$, any change to the terms in Q_2 will not effect the characteristic directions of the system.

Now let us examine the effects of a) ignoring the terms containing ϵ_x and b) including terms which contain a factor ρ/ρ_p . Case (a) is equivalent to setting D, G and J equal to zero. Immediately one can see that setting D and G equal to zero cannot effect the characteristic directions of the system because they appear only in Q_2 . Examination of Q_4 quickly shows that J does not enter into the evaluation of the determinant and therefore its value doesn't effect the characteristic directions. The effect of neglecting ϵ_x on the compatibility equations is not quite as simple to see; however, after expanding the M_1 determinants one finds that setting this term equal to zero yields two distinct compatibility equations along $\frac{dx}{dt} = u_p$.

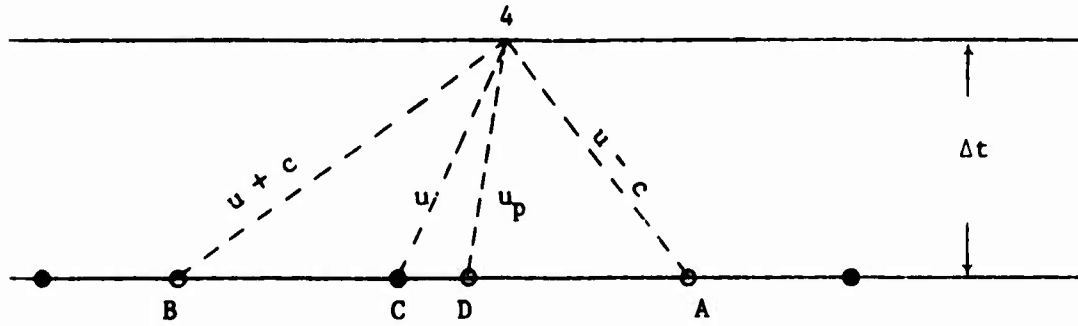
The inclusion of terms containing ρ/ρ_p , case (b), has the effect of altering Q_1 , Q_2 , Q_3 and Q_4 by adding a term involving the acceleration of the gas to the particle momentum equation, a term involving the acceleration of the particle to the gas momentum equation, and terms involving both accelerations to both the gas and particle energy equations. The determinant of the coefficient matrix, N, for this system is of the form:

$$N^* = \begin{vmatrix} dx-udt & -\sigma dt & 0 & 0 & 0 & 0 \\ -A dt & a_1(dx-udt) & -B dt & -D dt & a_2(dx-u_p dt) & 0 \\ 0 & c_2(dx-udt) & c_1(dx-udt) & -G dt & c_3(dx-u_p dt) & 0 \\ 0 & 0 & 0 & dx-u_p dt & -\sigma dt & 0 \\ 0 & b_1(dx-udt) & 0 & 0 & b_2(dx-u_p dt) & 0 \\ 0 & d_2(dx-udt) & 0 & 0 & d_3(dx-u_p dt) & d_1(dx-u_p dt) \end{vmatrix}$$

where the coefficients a_1 , a_2 , b_1 , b_2 , c_1 , c_2 , c_3 , d_1 , d_2 and d_3 are in general functions of the dependent variables. As can be seen, this system is quite a bit more complex than the one actually treated in this report. The expansion of N will result in a 6th order polynomial in $(dx/dt)^2$ which must be solved numerically to yield the characteristic directions. The number of real characteristic directions resulting from this equation is directly dependent on the values of the coefficients; thus, the nature of the system, at least conceptually, could change as the values of the dependent variables change. The derivation of the compatibility equations present a similar problem because they cannot be determined until the characteristic directions are known.

3. Finite Difference Form of the Compatibility Equations

The specific finite difference equations resulting from Eqs. (47) to (51) will now be presented. Referring to Fig. (12) we see that the locations where the characteristics emanating from the point being calculated, point 4, cross the previous time line, are labeled points A, B, C and D.



- - - - mesh points
○ - - - intermediate points (base of characteristics)

Figure 12. Characteristic network used in finite difference scheme

Utilizing the above point scheme and the notation that X_A corresponds to a property, X , evaluated at point A, X_{1A} corresponds to $(X_1)_A$ and Δt_A corresponds to Δt between points 4 and A: equation (47) solved for E_4 becomes

$$\begin{aligned}
 E_4 = E_C - \frac{1}{2} & \left[\frac{G_4 \sigma_{p4}}{(u_{p4} - u_4)^2} + \frac{G_C \sigma_{pC}}{(u_{pC} - u_C)^2} \right] (u_{p4} - u_{pC}) \\
 & - \frac{1}{2} \left[\frac{G_4}{(u_{p4} - u_4)} + \frac{G_C}{(u_{pC} - u_C)} \right] (\sigma_{p4} - \sigma_{pC}) + \frac{1}{2} \left[\frac{F_4}{\sigma_4} + \frac{F_C}{\sigma_C} \right] (\sigma_4 - \sigma_C) \\
 & + \frac{\Delta t_C}{2} \left[\frac{G_4 \sigma_{p4} PM_4}{(u_{p4} - u_4)^2} + \frac{G_C \sigma_{pC} PM_C}{(u_{pC} - u_C)^2} - \frac{G_4 PC_4}{(u_{p4} - u_4)} - \frac{G_C PC_C}{(u_{pC} - u_C)} \right. \\
 & \quad \left. + GE_4 + GE_C - \frac{F_4 GC_4}{\sigma_4} - \frac{F_C GC_C}{\sigma_C} \right] \quad (55)
 \end{aligned}$$

equation (48) solved for u_4 becomes

$$\begin{aligned}
 u_4 = u_B - \frac{1}{2} \left(\frac{Y_{14} \sigma_{p4}}{Y_{24}^2 c_4} + \frac{Y_{1B} \sigma_{pB}}{Y_{2B}^2 c_B} \right) (u_{p4} - u_{pB}) \\
 + \frac{1}{2} \left(\frac{Y_{14}}{Y_{24} c_4} + \frac{Y_{1B}}{Y_{2B} c_B} \right) (\sigma_{p4} - \sigma_{pB}) \\
 - \frac{1}{2} \left(\frac{B_4}{c_4} + \frac{B_B}{c_B} \right) (E_4 - E_B) - \frac{1}{2} \left(\frac{A_4}{c_4} + \frac{A_B}{c_B} \right) (\sigma_4 - \sigma_B) \\
 \frac{\Delta t_B}{2} \left(\frac{Y_{14} \sigma_{p4} PM_4}{Y_{24}^2 c_4} + \frac{Y_{1B} \sigma_{pB} PM_B}{Y_{2B}^2 c_B} - \frac{Y_{14} PC_4}{Y_{24} c_4} \right. \\
 \left. - \frac{Y_{1B} PC_B}{Y_{2B} c_B} + \frac{B_4 GE_4}{c_4} + \frac{B_B GE_B}{c_B} \right. \\
 \left. + GM_4 + GM_B + \frac{A_4 GC_4}{c_4} + \frac{A_B GC_B}{c_B} \right) \quad (56)
 \end{aligned}$$

where

$$Y_1 = G \times B + D \times c$$

and

$$Y_2 = u_p - u - c$$

equation(49)solved for σ_4 becomes

$$\begin{aligned}
 \sigma_4 = \sigma_A - \frac{1}{2} \left(\frac{Y_{34} \sigma_{p4}}{Y_{44}^2 A_4} + \frac{Y_{3A} \sigma_{pA}}{Y_{4A}^2 A_A} \right) (u_{p4} - u_{pA}) \\
 + \frac{1}{2} \left(\frac{Y_{34}}{Y_{44} A_4} + \frac{Y_{3A}}{Y_{4A} A_A} \right) (\sigma_{p4} - \sigma_{pA}) \\
 - \frac{1}{2} \left(\frac{B_4}{A_4} + \frac{B_A}{A_A} \right) (E_4 - E_A)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \left[\frac{c_4}{A_4} + \frac{c_A}{A_A} \right] (u_4 - u_A) \\
& + \frac{\Delta t_A}{2} \left[\frac{Y_{34} \sigma_{p4} PM_4}{Y_{44} A_4} + \frac{Y_{3A} \sigma_{pA} PM_A}{Y_{4A} A_A} \right. \\
& - \frac{Y_{34} PC_4}{Y_{44} A_4} - \frac{Y_{3A} PC_A}{Y_{4A} A_A} + \frac{B_4 GE_4}{A_4} \\
& \left. + \frac{B_A GE_A}{A_A} - \frac{c_4 GM_4}{A_4} - \frac{c_A GM_A}{A_A} + GC_4 + GC_A \right] \quad (57)
\end{aligned}$$

where

$$Y_3 = G \times B - D \times c$$

and

$$Y_4 = u_p - u + c$$

equation (50) solved for u_{p4} becomes

$$u_{p4} = u_{pD} + \frac{\Delta t_D}{2} (PM_4 + PM_D) \quad (58)$$

and Eq. (51) solved for σ_{p4} becomes

$$\begin{aligned}
\sigma_{p4} = \sigma_{pD} + \frac{\Delta t_D}{2} \left[PC_4 + PC_D - \sigma_{p4} \left(\frac{\partial u_p}{\partial x} \right)_4 \right. \\
\left. - \sigma_{pD} \left(\frac{\partial u_p}{\partial x} \right)_D \right] \quad (59)
\end{aligned}$$

Equations (55) to (59) are the equations used to calculate a regular point in our grid. Under certain conditions, however, they must be modified.

The first special case we will present occurs when the properties at points A,B,C and D are identical. When this occurs, Eqs. (47) to (51) reduce to

$$\begin{aligned}
du &= GM dt \\
d\sigma &= GC dt \\
dE &= GE dt \\
d u_p &= PM dt \\
d \sigma_p &= PC dt
\end{aligned}$$

These equations are finite differenced by averaging GM, GC, GE, PM, and PC between point 4 and point C.

The second special case occurs when either

$$u_{p4} - u_4 = 0$$

or

$$u_{pC} - u_C = 0$$

In this case the use of Eq. (55) would lead to a division by zero. Thus, we must finite difference Eq. (47) in the following form.

$$\begin{aligned} E_4 = E_C + \frac{1}{(u_{p4} - u_4 + u_{pC} - u_C)^2} & \left\{ (G_4 \sigma_{p4} + G_C \sigma_{pC}) \left[\frac{\Delta t_C}{2} (PM_4 + PM_C) \right. \right. \\ & - (u_{p4} - u_{pC}) \left. \right] - \left[G_4 (u_{p4} - u_4) + G_C (u_{pC} - u_C) \right] \\ & \times \left[\frac{\Delta t_C}{2} (PC_4 + PC_C) - (\sigma_{p4} - \sigma_{pC}) \right] - \left[\frac{F_{14} (u_{p4} - u_4)^2}{\sigma_4} \right. \\ & + \left. \frac{F_{1C} (u_{pC} - u_C)^2}{\sigma_C} \right] \left[\frac{\Delta t_C}{2} (GC_4 + GC_C) - (\sigma_4 - \sigma_C) \right] \left. \right\} \\ & + \frac{\Delta t_C}{2} (GE_4 + GE_C) \end{aligned}$$

4. Stability

We have conducted an investigation to gain insight into the stability of a mixed hyperbolic-parabolic system of equations such as we have here. Actually deriving a mathematically rigorous stability criterion for the highly non-linear equations of this report is quite a formidable task and not within the scope of this research. However, we feel that it is quite helpful to have an idea of the type of problems that might be encountered in treating our mixed system. It is our conclusion that the standard stability criterion for hyperbolic equations may not be sufficient for our system.

To demonstrate the above mentioned conclusion let us look at a particular system of equations for a problem coupling sound propagation and heat flow as presented by Richtmeyer [20], namely;

$$\frac{\partial u}{\partial t} = c \frac{\partial}{\partial x} (w + (\gamma-1)e)$$

$$\frac{\partial w}{\partial t} = c \frac{\partial u}{\partial x}$$

$$\frac{\partial e}{\partial t} = \sigma \frac{\partial^2 e}{\partial x^2} - c \frac{\partial u}{\partial x}$$

where u is the material velocity, $w = c V/V_0$, V is the specific volume, $e = E/c$, E is the specific internal energy, c is the isothermal sound speed, and σ is the ratio of thermal conductivity to specific heat at constant volume. These equations are formed by coupling the hyperbolic fluid dynamic equations to the parabolic heat flow equations. The first two equations above may be said to be hyperbolic in nature, while the third is parabolic in nature. An analogous situation occurs with the equations of this report where Eqs. (1), (2) and (3) are hyperbolic in nature, and Eqs. (4) and (5) are parabolic in nature.

Without going into the finite differencing details which are presented on page 171 of [20] we will proceed right to the conclusions concerning the stability. Although a precise stability criterion for this complete system was not found, Ref. [20] states that it is surely necessary for it to satisfy the stability criteria of both the uncoupled fluid dynamics equations and the uncoupled heat flow equation. The stability criteria for these two systems are respectively:

$$\frac{\sqrt{\gamma} c \Delta t}{\Delta x} < 1$$

and

$$\frac{\sigma \Delta t}{(\Delta x)^2} < \frac{1}{2}$$

It is also stated that in the limit, as Δx and Δt go to zero, the second condition implies the first and thus is assumed to be the stability criterion for the system.

This example demonstrates the possibility that a mixed hyperbolic parabolic system may be finite differenced in such a manner as to yield a stability criterion which is directly dependent on the parabolic segment of the equations. With this in mind let us examine the possibilities that exist for our system of equations.

a. The hyperbolic stability criterion dominates and is given by

$$(|u| + c) \frac{\Delta t}{\Delta x} \leq K$$

or

$$\Delta t \leq \frac{K \Delta x}{(|u| + c)} \leq K_1$$

where K is equal to 1.

When this criterion is programmed, the value of K is set somewhat less than 1 to allow for the fact that the properties on the new time line are unknown when Δt is calculated and must be estimated.

b. The parabolic stability criterion dominates and is of the same form as the hyperbolic criterion. This criterion is programmed in the same manner as the hyperbolic criterion except that K may now be significantly less than 1.

c. The third possible criterion results from the comparison of the parabolic segment of our system with the heat flow equation in Sec. (II,4). It can be shown that from a characteristic standpoint the roles of x and t are reversed between the two systems. The stability criterion for the heat flow equation is of the form

$$\frac{\Delta t}{\Delta x^2} < K_2^2$$

which leads to the possibility that the stability criterion for our parabolic equations may take the form

$$\frac{\Delta t^2}{\Delta x} > K_2^2$$

or

$$\Delta t > K_2 (\Delta x)^{1/2} = K_3$$

If K_3 is less than K_1 then a value of Δt may be chosen such that

$$K_3 < \Delta t < K_1$$

However, if K_3 is greater than K_1 no value of Δt will satisfy both the hyperbolic and parabolic stability criterion and the system is unconditionally unstable.

All indications from past research are that this last case does not exist; Rudinger [10] and Rudinger and Chang [11] have solved systems of equations which are quite similar to those presented here and have not reported stability problems. It is felt that, although care must be taken in running the code, selection of Δt to achieve stability can be achieved by using the stability criterion of a. and allowing K to vary between 0 and 1.

5. General Point Iteration Procedure

The most difficult portion of the computer code is centered on the solution of Eqs. (55) to (59). At first a simple procedure was tried where, each equation is solved for one particular variable, then updated by averaging the most recent value with the old value utilizing a relation of the form

$$u_{n+1} = \frac{u_n + BK \times u_{n-1}}{AK} \quad (60)$$

where the values of AK and BK can be adjusted at the programmers discretion. This proved unsuccessful, causing rapid divergence of the system. Upon close examination of the equations, it was felt that the best hope for solution would be to uncouple the gas and particle phases and solve Eqs. (55), (56) and (57) as a set and Eqs. (58) and (59) as a set. This is accomplished by assuming that the particle properties are constant while solving Eqs. (55), (56) and (57) and conversely the gas properties are constant when solving Eqs. (58) and (59). Even making this assumption, the solution of Eqs. (55), (56) and (57) for the gas properties is a quite formidable task due to the high degree of nonlinearity. It was decided to solve these three equations for the variables σ , u and E using the Newton-Raphson technique. Before proceeding, it should be noted that Eq. (55) is linear in the variable E and can be written in the form

$$E = E(u, \sigma) \quad (61)$$

Thus conceptually, Eqs. (56) and (57) when combined with (61) can be written in the form

$$g(u, \sigma) = 0 \quad (62)$$

$$f(u, \sigma) = 0 \quad (63)$$

respectively. The Newton Raphson procedure for two equations can then be utilized, namely

$$u_{n+1} = u_n + \Delta u \quad (64)$$

and

$$\sigma_{n+1} = \sigma_n + \Delta \sigma \quad (65)$$

where

$$\Delta u = \left(f \frac{\partial g}{\partial \sigma} - g \frac{\partial f}{\partial \sigma} \right) / XJ$$

$$\Delta \sigma = \left(g \frac{\partial}{\partial} - f \frac{\partial g}{\partial u} \right) / XJ$$

$$XJ = \frac{\partial f}{\partial \sigma} \frac{\partial g}{\partial u} - \frac{\partial f}{\partial u} \frac{\partial g}{\partial \sigma}$$

Before applying this technique further convenient simplifications were made. They are as follows:

- a. along with holding the particle properties constant we decided to also hold p and c constant. This assumption was more or less made out of necessity due to the difficulty in evaluating the partial derivatives of g and f .
- b. Provision was made and subsequently adopted to hold the values of GC , GM , GE , PC , PM constant through this sub iteration.

Having made these assumptions preliminary calculations produced rapid convergence of the Newton-Raphson routine and subsequent convergence of the entire general point routine by then solving Eq. (58) for u_p and Eq. (59) for σ_p and then correcting the entire set of solutions using equations of the form (60) with $AK = 2$ and $BK = 1$.

The calculations proceeded routinely for many time lines utilizing this technique; however, as the value of u_p started to approach u (particles became small) the solution to the system of equations began to diverge. To better understand the cause of this problem and the necessary steps to correct it the entire system of equations was closely examined. It was found that the trouble was rooted in the solution of Eqs. (55), (56) and (57) and more specifically in Eq. (55). To analyze this problem we will write Eq. (55) in a general form, namely:

$$E = \frac{f_1(u, \sigma)}{(u_p - u)^2} (du_p - PMdt) + \frac{f_2(u, \sigma)}{(u_p - u)} (d\sigma_p - PCdt) + f_3(u, \sigma) \quad (66)$$

Now let us examine a term of the nature $(u_p - u)^m$ ($m = -1, -2$) in context with our iteration procedure noting that u_p is constant. To do this it is simplest to forsake rigor and go directly to a typical numerical example. First let us assume a problem where the difference between u_p and u is large; such as:

$$u_p = 10$$

$$u = 100$$

Now let us see what happens to the coefficient of the first term on the right hand side of Eq. (61), which we will call F_1 , if u varies by, let us say 2 from one iteration to the next, i.e. Δu in Eq. (64) is equal to 2.

- 1) for $u = 100$ we have

$$F_1^{100} = \frac{f_1^{100}}{8100}$$

- 2) for $u = 102$ we have

$$F_1^{102} = \frac{f_1^{102}}{8464}$$

assuming that $f_1^{100} \approx f_1^{102}$ which in reality is pretty close to being true we have a percent change in F_1 of approximately 4%.

For our second example let us assume a problem where the difference between u_p and u is small such as

$$\begin{aligned} u_p &= 95 \\ u &= 100 \end{aligned}$$

Now again let us assume that u varies by 2 from one iteration to the next and examine F_1 or

$$1) \quad \text{for } u = 100$$

$$F_1^{100} = \frac{f_1^{100}}{25}$$

$$2) \quad \text{for } u = 102$$

$$F_1^{102} = \frac{f_1^{102}}{49}$$

Making the same assumptions on f_1 as in the previous example we can see that the change in F_1 is now approximately 50%. It turns out that this rapid change in F_1 causes the entire Newton-Raphson technique to become unstable.

The problem now centers on what steps should be taken to correct this deficiency. It is quite obvious that we cannot tolerate "large" changes in u during an iteration when the values of u and u_p are "close". One approach to the problem would be to attempt to improve the first guess; however, first guesses consisting of the base point properties and the solution of the linearized system of equations proved unsuccessful and this approach was abandoned.

The approach that proved successful is as follows. First, attempt to solve the complete set of equations. If this fails, set f_1 equal to zero and solve that set of equations. Then use its solution, after having corrected E_4 by adding the f_1 term back in, as a first guess in solving the complete set. If this still fails, set both f_1 and f_2 equal to zero and follow the same procedure.

The degree to which the solution of the equations with f_1 set equal to zero approximates the solution to the complete set is related to how close the term $(du_p - PMdt)$ is to zero. Notice that this term is in the same form as Eq. (35) the only difference being that Eq. (61) is written along $dx/dt = u$ and Eq. (35) along $dx/dt = u_p$.

Thus it can be easily seen that as u_p approaches u , the term $(du_p - PMdt)$ written along $dx/dt = u$ approaches zero and the solution of the simplified system approaches the solution of the complete system. In summary, it should be noted that although the term $(du_p - PMdt)$ is approximately equal to zero when the system converges, during the iteration procedure it can become quite large and cause convergence problems.

IV. Results and Discussions

Before presenting a complete test run for the M16 rifle, we will briefly point out two features of the code TWOFL0 which are not treated by other codes. The first feature is the treatment of a gas only region behind the bullet. A typical plot of ϵ and u vs. time in the vicinity of the interface between this gas only region and the two phase flow region is shown in Fig. (13).

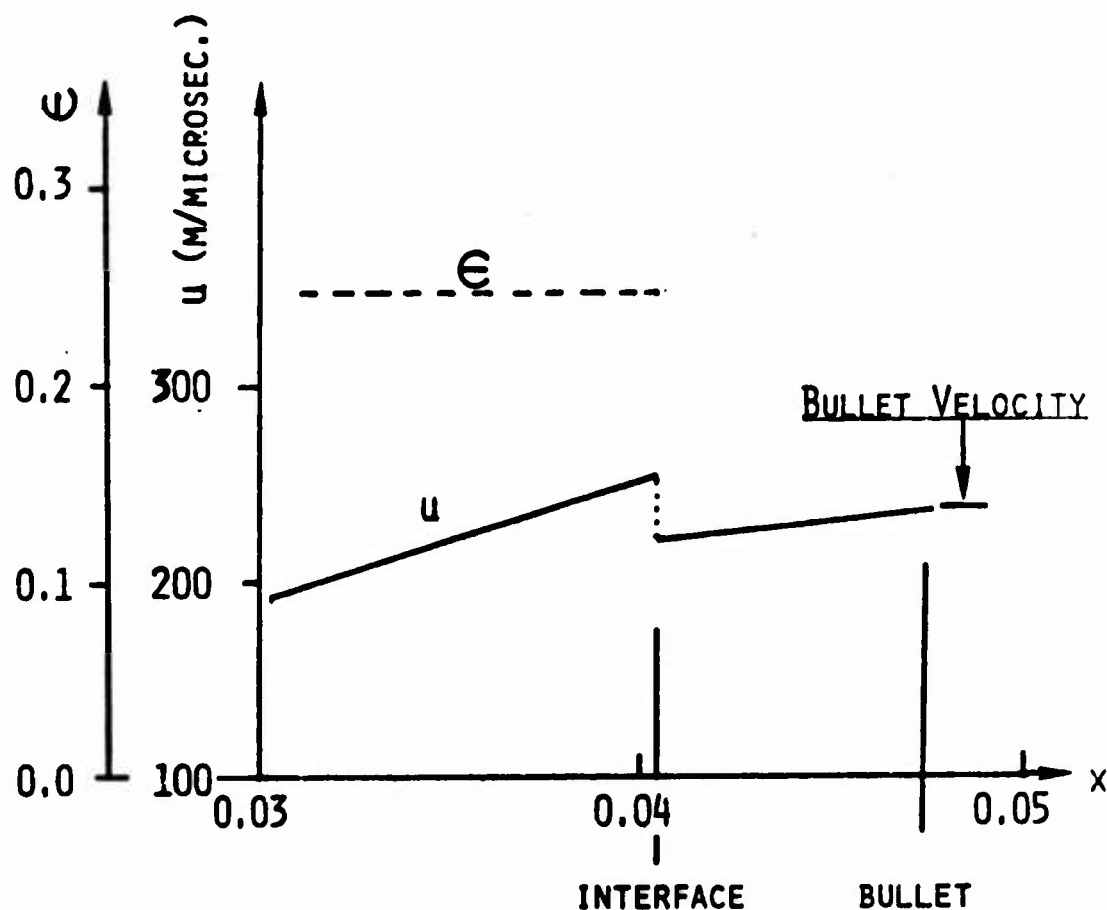


Figure 13. Plot of loading, ϵ , and gas velocity, u , vs. distance from the breach, x .

Notice that at this interface there is a discontinuity in ϵ leading to a discontinuous drop in particle velocity. The second feature deals with a shock wave traveling behind the bullet. Figure (14) shows a plot of the physical plane and a plot of pressure vs. position as the shock passes through the gas-particle interface. Referring to the pressure curve in Fig. (14) one can see that the effects of the contact line have been neglected and the rarefaction wave has been smoothed out consistent with the discussion in Sec. (II,7)

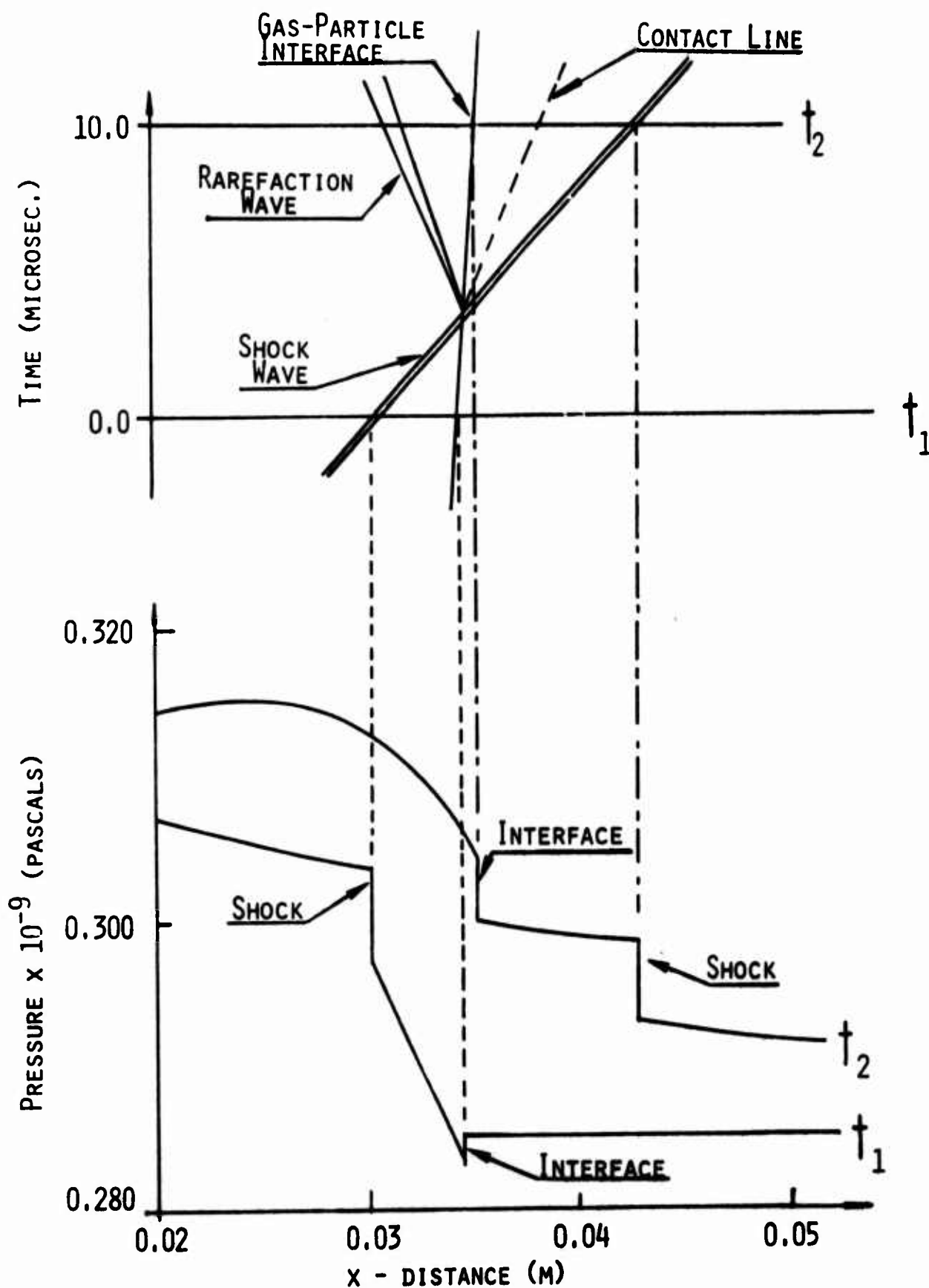


Figure 14. Plot of TWOFL0 calculations for a right traveling shock wave passing through a gas-particle interface.

Presented next are numerical results for the M16 rifle beginning at the time of complete ignition and extending until the bullet leaves the barrel.

Two separate runs were made each with a different size propellant particle. The propellant used is pancake shaped, $(1.814 \times 10^{-3} \text{ Kg of WC 846})$. The drag force between the particles and the gas is approximated by that of a sphere having the same radius as the radius of the pancake. The propellant was assumed to be compacted by the initial primer blast. This is treated in the code by shortening the rear of the cartridge by 0.005m. The loading after compaction, ϵ , was 0.575. Other pertinent data for these runs can be found in the sample input section of Appendix C.

The sizes of the propellant particle used for the runs are summarized as follows:

	Particle Radius	Particle Thickness
RUN A	$2.730 \times 10^{-4} \text{ m}$	$3.810 \times 10^{-4} \text{ m}$
RUN B	$1.365 \times 10^{-4} \text{ m}$	$1.905 \times 10^{-4} \text{ m}$

For Run A the particle dimensions conform to the average dimensions of the actual propellant. The particle size of Run B is one-half of that of Run A. Run B was chosen to determine the effect of increasing the propellant surface area. The calculated results for these two cases are compared with the experimental results of Trafton [28].

Figure (15) shows the velocity of the bullet plotted against the distance from the base of the cartridge. Run A yields a muzzle velocity that is 35% lower than the experimental one; Run B produced a much higher muzzle velocity, but is still 17% lower than the experimental value

Examining Fig. (16) one can see that the pressure produced at the midpoint of the chamber by Runs A and B brackets the experimental values fairly well, noting that the 300 μsec time duration for complete ignition to occur (this represents the time between primer ignition and the initiation of TWOFL0 calculations) is not exact; any error in this time would shift the pressure curves horizontally. Although Run B produces pressure higher than the experimental value at a station in the chamber, it produces a much lower pressure at a station further downstream in the barrel, as shown in Fig. (17).

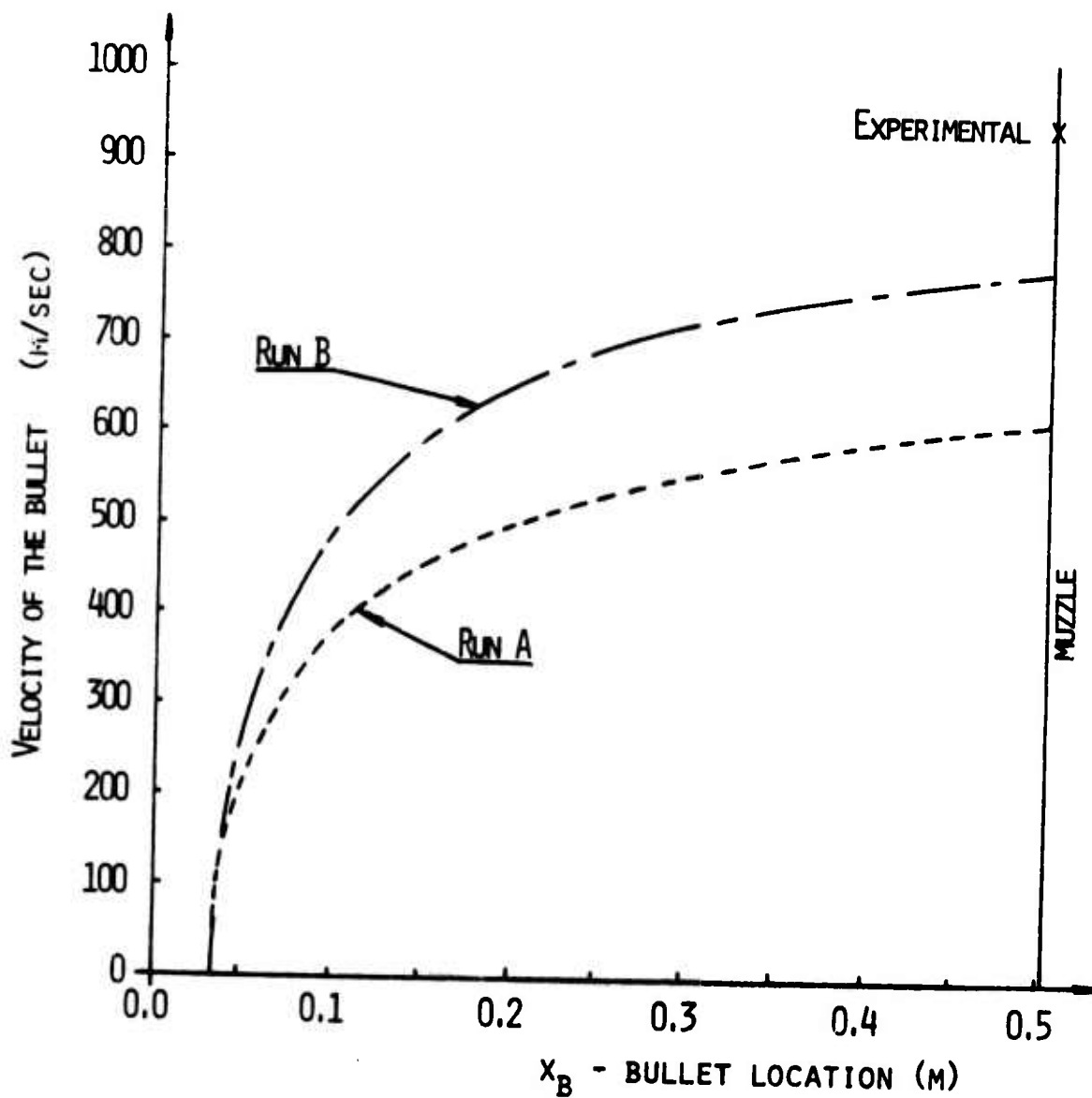


Figure 15. Plot of x_B (location of bullet measured from the breech) vs. bullet velocity.

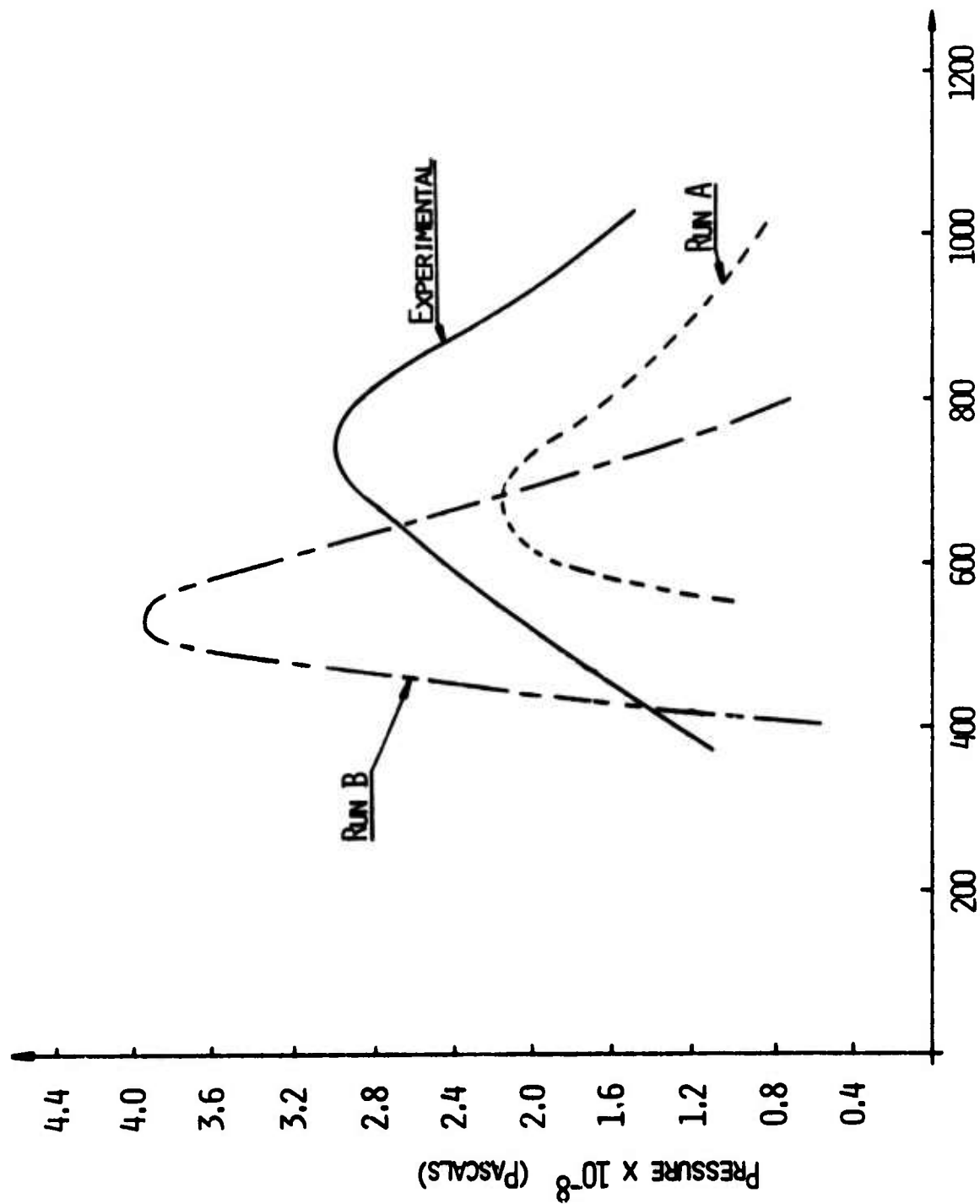
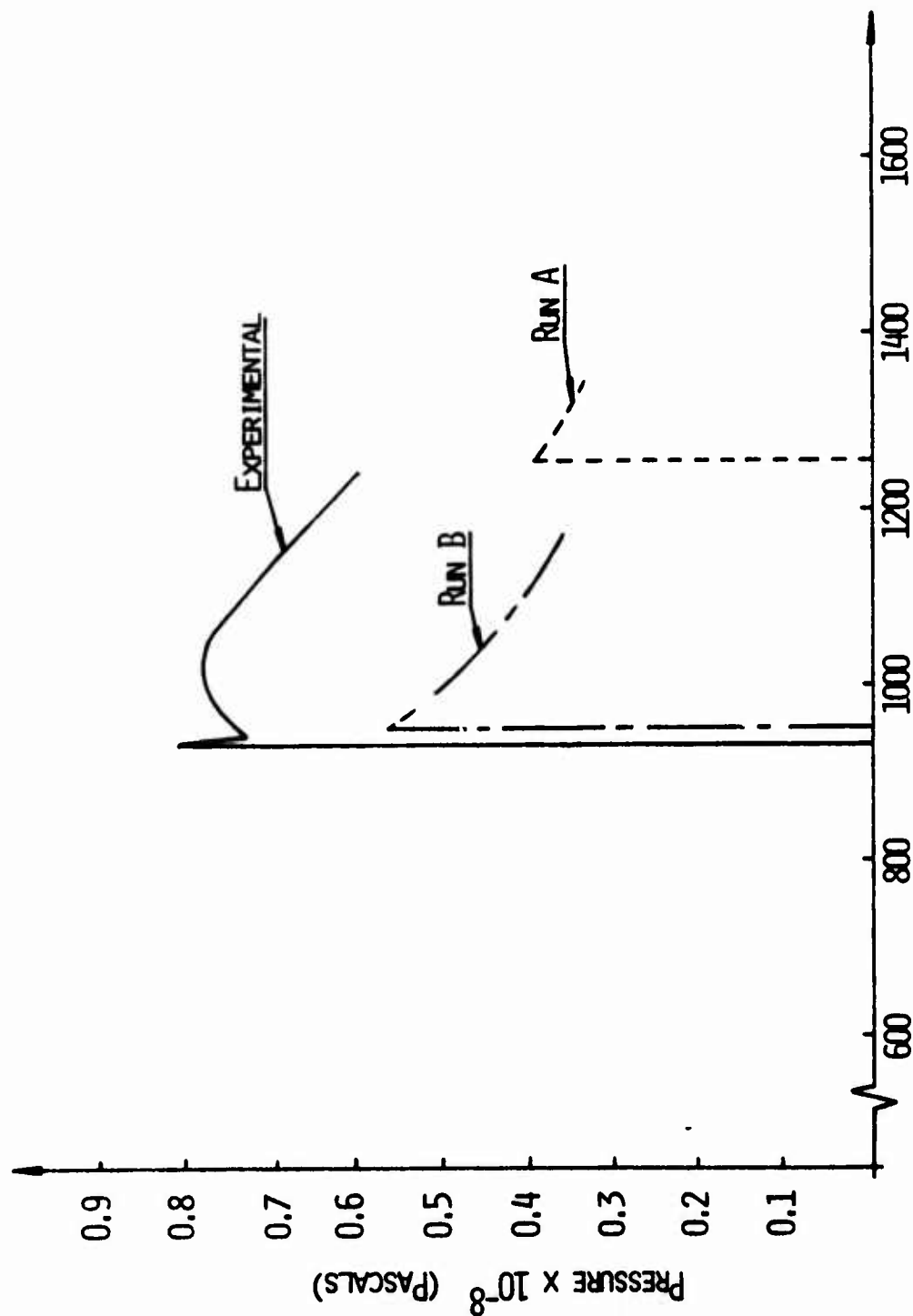


Figure 16. Plot of pressure vs. time from ignition at a point located at the mid point of the chamber (0.014m from base of the cartridge).



TIME FROM PRIMER IGNITION (ASSUME 300 MICRO SEC. FOR COMPLETE IGNITION) (MICRO SEC.)

Figure 17. Plot of pressure vs. time from ignition at a point located at the gas port (0.328m from the base of the cartridge)

Fig. (17) is a plot of pressure vs. time at the gas port, substantially down the barrel. By this time, both Runs A and B produce pressures that are substantially below the experimental results. These results seem to indicate that too large of a portion of the energy, as computed by TWOFLO, remains in the rear section of the barrel whereas it should be more concentrated near the bullet.

There are two possible reasons for the discrepancy between the calculated and experimental results. The first is the uncertainty about the physical parameters used as input data in the calculation. These include the burning rate of the propellant, the drag coefficient of particles, ignition time, the state at the end of the ignition process, the friction between the bullet and the barrel, etc. Hopefully, a computer code that is numerically accurate, together with certain easily measured physical parameters, can be used to determine all the other parameters, in the future.

The other possible reason is the inaccuracy of the code, either in the governing equations used, or in the numerical solution of these equations. Preliminary test calculations show that the numerical solution converges; solutions from using two different mesh sizes vary very little. Calculation of a simple one-phase flow problem also indicates that results are very close to the exact solution. Therefore, we have confidence in the numerical accuracy.

As discussed in Appendix A, the governing equations used involve certain approximations. In particular, a term in the particle momentum equation has been neglected for simplicity in applying the method of characteristics. This term is relatively small for small values of ϵ , but can become important for large value of ϵ . It can be seen from Eq. (A12) that by neglecting this term, we decreased the particle acceleration. This might have contributed to the slower motion of the particles, and the concentration of energy and pressure near the chamber.

For further development of this work, we suggest the following:

- a. Modification of Governing Equations - Although the equations we used are quite elaborate and include many more terms than most earlier works, preliminary numerical results indicate that certain neglected terms should be retained. For instance, the Du/Dt term in the particle momentum could be retained.
- b. Complete Test Runs - Appropriate sample problems should be run with the code to ascertain the convergence and stability of the numerical calculation. Comparison with simpler problems with exact solutions, and with other numerical methods should be made. A parametric study to determine the importance of various terms in the equations, and the effect of certain physical quantities would also be desirable.

- c. Comparison with Experimental Results - This type of comparison can serve to determine the accuracy of the calculated results if the experimental results are accurate, or vice versa.
- d. Solve a Problem with Shock Waves - This code has the capability to treat shock waves; shocks are traced exactly, instead of being smeared by artificial viscosity as in finite-difference methods. The subroutines are all debugged, but have not been tried out on a physical problem with shocks. This should be done.

In conclusion, the following points about the TWOFLO code can be made.

- 1. It is one of the most "sophisticated" one-dimensional codes. It treats the two phases separately, includes the effects of wall area change, wall friction, heat and mass transfer through the wall, includes the $\partial \epsilon / \partial x$ effect, etc. The governing equations include many additional terms as compared with other existing codes.
- 2. It is accurate. TWOFLO incorporates the method of characteristics, which is inherently more accurate than the finite-difference method. It handles the initial and boundary conditions in a logical manner.
- 3. It has the capability of treating shock waves. Shocks are traced exactly. For those physical problems where shocks are present, this code can yield more accurate results. Even in problems without shocks, the characteristic lines and contact lines calculated from this code can reveal more about the nature of the flow.

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APPENDIX A-DERIVATION OF TWO PHASE FLOW GOVERNING EQUATIONS*

In deriving the governing equations for this system let us treat the gas phase and the particle phase separately while coupling their motion through interaction terms. When treating each phase, we will assume that it forms a continuum and occupies the entire control volume at a given instant. In utilizing this concept, we must replace the classical density which represents mass per unit volume, with a new term representing mass per unit volume of mixture. We will also assume that the particles are rigid and that they may be considered to be large with respect to the molecular size of the gas and thus do not contribute to the pressure of the mixture. Having taken these assumptions into consideration, we may write the governing equation for each component of the mixture.

1. Continuity equations

The continuity equation for the gas phase can be obtained by establishing a control volume and equating the time rate of increase of mass inside the control volume to the time rate of mass added to the control volume, where the mass added is composed of three terms; the net mass flux into the control volume through the end surface normal to the flow, the mass addition resulting from the particles burning and the mass transport through the wall, or

$$\frac{\partial(\sigma A)}{\partial t} = - \frac{\partial(\sigma u A)}{\partial x} + (\omega A) - (\omega_w A) \quad (A1)$$

which can be rearranged as

$$\frac{D\sigma}{Dt} + \sigma \frac{\partial u}{\partial x} = - \frac{\sigma u}{A} \frac{dA}{dx} + \omega - \omega_w \quad (A2)$$

Similarly, the continuity equation for the particle phase is

$$\frac{\partial(\sigma_p A)}{\partial t} = - \frac{\partial(\sigma_p u_p A)}{\partial x} - (\omega A) - (\omega_{wp} A) \quad (A3)$$

which can also be rearranged, producing

$$\frac{D\sigma_p}{Dt} + \sigma_p \frac{\partial u_p}{\partial x} = - \frac{\sigma_p u_p}{A} \frac{dA}{dx} - \omega - \omega_{wp} \quad (A4)$$

2. Momentum equations

Before proceeding to derive the momentum equations we will make several additional assumptions, namely:

* We would like to make a special acknowledgement to Dr. Aivars Celmins who made an invaluable contribution in the formulation of the equations in this Appendix.

- a. When mass transfer occurs between the phases, the particle phase always loses mass, the gas phase always gains mass; or $\omega \geq 0$.
- b. The gas and particle phases may discharge through the wall, but injection is not treated, or

$$\omega_w \geq 0; \quad \omega_{wp} \geq 0.$$

When leakage occurs, the gas and particle phases lose mass that is moving at velocities of u_w and u_{wp} respectively. One possible assumption is to consider the discharged mass having the same axial velocity as the "parent" media. This is justified by the fact that within the flow field our one-dimensional assumption does not account for variations in velocity across the cross-section.

- c. During the burning process the gas phase gains momentum equal to ωu_p while the particle phase loses the same amount.

Having made these assumptions we will now derive the momentum equation for the gas phase which equates the time rate of increase of momentum in a control volume, to the forces acting on the control volume (positive if acting in the positive x direction). These forces include the reaction of the net momentum flux through the main entrance and exit of the control volume, the force due to the momentum flux associated with mass addition from burning, the reaction due to momentum loss associated with mass passing through the wall, the pressure gradient force, the interaction force of the particles acting on the gas and the force from the outside wall, or

$$\frac{\partial(\sigma Au)}{\partial t} = -\frac{\partial(\sigma Au^2)}{\partial x} + \omega u_p A - (\omega_w u_w A) - A \frac{\partial p}{\partial x} - \bar{F}A + F_w A \quad (A5)$$

where the term u_w is the x component of velocity of the gas leaving the control volume through the wall.

Equation (A5), after combining with the gas continuity equation, Eq. (A2), can be written as

$$\sigma \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + F_w - \bar{F} + \omega(u_p - u) - \omega_w(u_w - u) \quad (A6)$$

Similarly, the momentum equation for the particle phase is

$$\frac{\partial(\sigma_p A u_p)}{\partial t} = \frac{\partial(\sigma_p A u_p^2)}{\partial x} - (\omega u_p A) - (\omega_{wp} u_{wp} A) + \bar{F}A + F_{wp} A \quad (A7)$$

which upon simplification becomes

$$\sigma_p \frac{D^p u_p}{Dt} = F_{wp} + \bar{F} - \omega_{wp} (u_{wp} - u_p) \quad (A8)$$

where the term u_{wp} is the x component of the velocity of the particles passing through the wall.

In Eqs. (A6) and (A8), the interaction force between the gas and the particles, \bar{F} , in general, includes four types of forces, namely, the viscous drag force, the pressure gradient force, the apparent mass force due to the acceleration of the gas surrounding the particles and the force due to nonsteady flow. Note that the drag force does not include the pressure gradient effect. Often, the drag force determined experimentally contains both the effects of viscosity and pressure. Special care must be taken to separate these effects in using the present set of equations. A detailed discussion on these forces may be found in Hinze [A1], Rudinger [A2], Pai [A3] and Willis [A4]. Let us follow the approach of Hinze, and consider the force acting on a spherical particle, given by

$$F_s = C_D \frac{\pi D^2}{8} \rho |u - u_p| (u - u_p) - \frac{\pi D^3}{6} \frac{\partial p}{\partial x} + \frac{1}{2} \frac{\pi D^3}{6} \rho \left(\frac{Du}{Dt} - \frac{D^p u_p}{Dt} \right) + \frac{3}{2} D^2 \sqrt{\pi \rho \mu} \int_0^t \left(\frac{Du}{Dt} - \frac{D^p u_p}{Dt} \right) (t - \tau)^{-1/2} d\tau$$

If we now define the number of particles per unit volume of mixture, N , as

$$N = \frac{\sigma_p}{\rho_p \times (\text{Volume of a particle})} = \frac{6\epsilon}{\pi D^3}$$

then

$$\begin{aligned}
 \bar{F} &= N \times F_s \\
 &= \epsilon \left[\frac{3C_D \rho}{4D} |u - u_p| (u - u_p) - \frac{\partial p}{\partial x} - \frac{1}{2} \rho \left(\frac{Du}{Dt} - \frac{D^p u_p}{Dt} \right) \right. \\
 &\quad \left. + \frac{9}{D} \sqrt{\frac{\mu \rho}{\pi}} \int_0^t \left(\frac{Du}{D\tau} - \frac{D^p u_p}{D\tau} \right) (t - \tau)^{-1/2} d\tau \right] \\
 &= -\epsilon \frac{\partial p}{\partial x} + F
 \end{aligned} \tag{A9}$$

where F represents the interaction force without the pressure gradient term. As the value of $\frac{\rho}{\rho_p}$ becomes small, the apparent mass force and the force due to nonsteady flow become negligible. It is assumed for the problem presented here that the values of ρ/ρ_p encountered are small enough so that these terms can be neglected leaving us with an expression for F which includes only the viscous drag force, namely:

$$F = \frac{\rho}{\rho_p} K_1 |u - u_p| (u - u_p)$$

where

$$K_1 = \frac{3C_D \sigma_p}{4D}$$

Setting u_w equal to u and u_{wp} equal to u_p , Eqs. (A6), (A8) and (A9) combine to become

$$\frac{Du}{Dt} + \frac{(1-\epsilon)}{\sigma} \frac{\partial p}{\partial x} = -\frac{1}{\sigma} [(F - F_w) - \omega(u_p - u) + \omega_w(u_w - u)] \tag{A10}$$

and

$$\frac{D^p u_p}{Dt} + \frac{\epsilon}{\sigma_p} \frac{\partial p}{\partial x} = \frac{1}{\sigma_p} [(F_{wp} + F) - \omega_{wp}(u_{wp} - u_p)] \tag{A11}$$

respectively. Solving eq. (A10) for $\frac{\partial p}{\partial x}$ and substituting into Eq. (A11) yields:

$$\begin{aligned}
 \frac{D^p u_p}{Dt} - \frac{\rho}{\rho_p} \frac{Du}{Dt} &= \frac{1}{\sigma_p} \left\{ F_{wp} + F + \frac{\epsilon}{(1-\epsilon)} [F - F_w - \omega(u_p - u)] \right. \\
 &\quad \left. + \omega_w(u_w - u) - \omega_{wp}(u_{wp} - u_p) \right\}
 \end{aligned} \tag{A12}$$

The term $\frac{\rho}{\rho_p} \frac{Du}{Dt}$ will now be neglected for simplicity. With this term neglected, the particle equations are weakly coupled to the system, i.e., the particle equations do not contain derivatives of the gas variables u , σ , and E . The ratio of this term over the first term of A12 is

$$\frac{\frac{\rho}{\rho_p} \frac{Du}{Dt}}{\frac{D^p u_p}{\rho_p \frac{D^p u_p}{Dt}}} = \frac{-\frac{\partial p}{\partial x} + \frac{1}{1-\epsilon} (F_w - F)}{-\frac{\partial p}{\partial x} + \frac{1}{\epsilon} (F + F_{wp})}$$

which is much less than one when ρ/ρ_p and ϵ are both small. For instance, in the numerical example treated later, this ratio is less than 0.15 for most points in the flow field. However, near the breech and during the time immediately after initiation, this ratio may be larger than 0.5 and the omission of the Du/Dt term may be a poor approximation. An attempt should be made to retain this term in future refinement of this work. Eq. (A8) is then reduced to

$$\frac{D^p u_p}{Dt} = \frac{1}{\sigma_p} \left\{ \frac{\epsilon}{1-\epsilon} [(F-F_w) - \omega_p(u_p-u) + \omega_w(u_w-u) + (F + F_{wp}) - \omega_{wp}(u_{wp}-u_p)] \right\} \quad (A13)$$

Equations (A10) and (A13) are the momentum equations used in the computer code for the gas and particle phases respectively.

In the derivation leading to Eq. (A10), we have implied that the pressure force acting on the particles is $-\epsilon \partial p / \partial x$, which is different from Pai's expression of $-\partial(p\epsilon)/\partial x$. We feel that our approach is more realistic for the present problem. In order to get a better feel for this term let us examine in more detail the pressure force acting on the particles and compare our approach to Pai's [A3]. Let us begin by discussing Pai's treatment of the pressure itself. In his approach, he assumes that the particle density ρ_p is constant (the particle concentration σ_p is variable) and that the pressure of the mixture p , which he calls total pressure, is the true pressure of the gas. He defines the gas partial pressure, p_g , as the pressure of the gas of fixed mass and fixed temperature, if it were to occupy the entire volume of the mixture. If the equation of state of the gas is

$$p = p(\rho, E) \quad (A14)$$

then p_g is defined by,

$$p_g = (\sigma, E) = p[\rho(1-\epsilon), E] \quad (A15)$$

In addition, if the pressure is a linear function of ρ ($p = \rho f(E)$) which is the case for an ideal gas, then p_g is given by

$$p_g = (1-\epsilon) \rho f(E) = (1-\epsilon)p \quad (A16)$$

The total pressure of the mixture is considered as the sum of the partial pressure of the gas, p_g , and that of the pseudo-fluid of particles, p_p or

$$p = p_g + p_p$$

From the above, it follows that

$$p_p = \epsilon p$$

Note that the definition of the partial pressure of the gas, p_g , follows Dalton's law of partial pressure, i.e. the partial pressure of a component in a mixture is the pressure that the component would exert if it were alone in the container. However, in reality, partial pressure of the particle phase p_p , does not obey Dalton's law, i.e. if the particles were alone in the container they would not produce a pressure.

Now, we will proceed to discuss the pressure force acting on each phase. In Pai's approach, the particles are considered to be smeared and occupy the complete volume of the mixture, with only their partial pressure, p_p , acting on them. In our approach, we also consider the particles to be smeared; however, we assume that they occupy only a portion of the volume having an effective cross-sectional area which is being acted upon by the total pressure.

The particle equation of motion as derived by Pai is of the form, (the following discussion also holds for the gas)

$$\sigma_p \frac{D u_p}{Dt} + \frac{\partial p}{\partial x} = \text{---}, \text{ where the right hand side contains no derivatives.}$$

The pressure gradient term in this equation can be written as $\frac{\partial(\epsilon p)}{\partial x}$ which is different from that in our equation of motion, $\epsilon \frac{\partial p}{\partial x}$.

In other words, we do not include the term $p \frac{\partial \epsilon}{\partial x}$ in our equation of motion. We can justify this by analyzing the following models. However, first, let us review the derivation of the momentum equation for a single phase flow with area change.

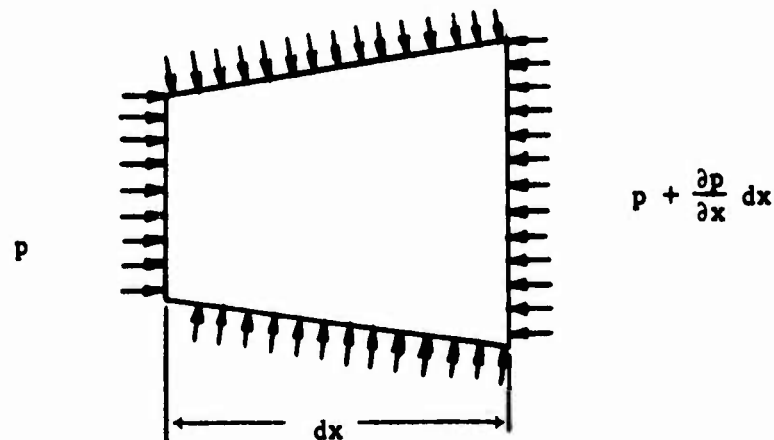


Figure A1 - Control Volume of a Single Phase Flow

Considering the control volume shown in Fig. (A1), the net pressure force, p_n , acting on this control volume is in the x direction and given by

$$p_n = + p A + (p + \frac{\partial p}{\partial x} \frac{dx}{2}) \frac{dA}{dx} dx - (p + \frac{\partial p}{\partial x} dx)(A + \frac{dA}{dx} dx)$$

where the second term on the right hand side is the pressure force on the side wall. After neglecting terms of second order in dx , the above equation becomes

$$p_n = - A \frac{\partial p}{\partial x} dx.$$

Note that there are no first order contributions from the change in area $\frac{dA}{dx}$ to the net pressure force; the first order effect of the pressure $\frac{dp}{dx}$ force due to $\frac{dA}{dx}$ on the right-hand surface is cancelled by the pressure force on the side wall.

For the particles in a two-phase flow we have a similar situation (Fig. A2). Let A be the cross-sectional area of the mixture, $\epsilon_1 A$ be the equivalent cross-section area of the particles, and $\epsilon_2 dx$ be the equivalent length of the particles such that $\epsilon_1 \epsilon_2 = \epsilon$,

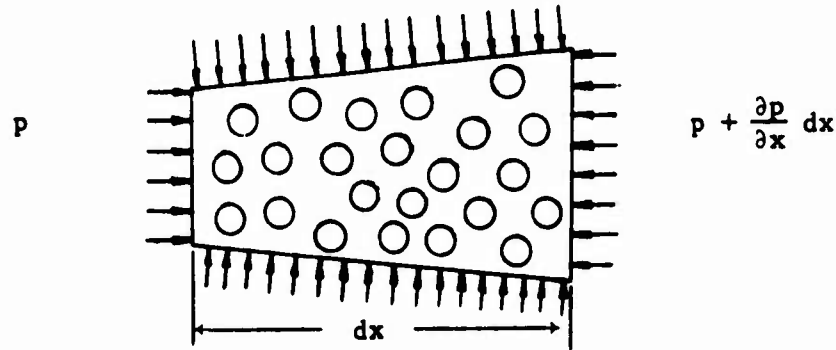


Figure A2 - Control Volume for a Particle -
Gas Two-Phase Flow

The net pressure force on the particles is then

$$p_n = p \epsilon_1 A + (p + \frac{\partial p}{\partial x} \frac{\epsilon_2 dx}{2}) \frac{\partial(\epsilon_1 A)}{\partial x} dx - (p + \frac{\partial p}{\partial x} \epsilon_2 dx) \left[\epsilon_1 A + \frac{\partial(\epsilon_1 A)}{\partial x} \epsilon_2 dx \right]$$

which after neglecting second order effects becomes

$$p_n = - \frac{\partial p}{\partial x} A \epsilon dx.$$

Note that in our formulation, we treat the change in ϵ as a change in area, resulting in a net pressure force on the particles that does not include a term of the form $\frac{\partial \epsilon}{\partial x}$.

The same conclusion may also be reached by considering an extreme case, where all of the particles are concentrated in a "rod" of area $A\epsilon$ and length dx , as shown in Fig. A3.

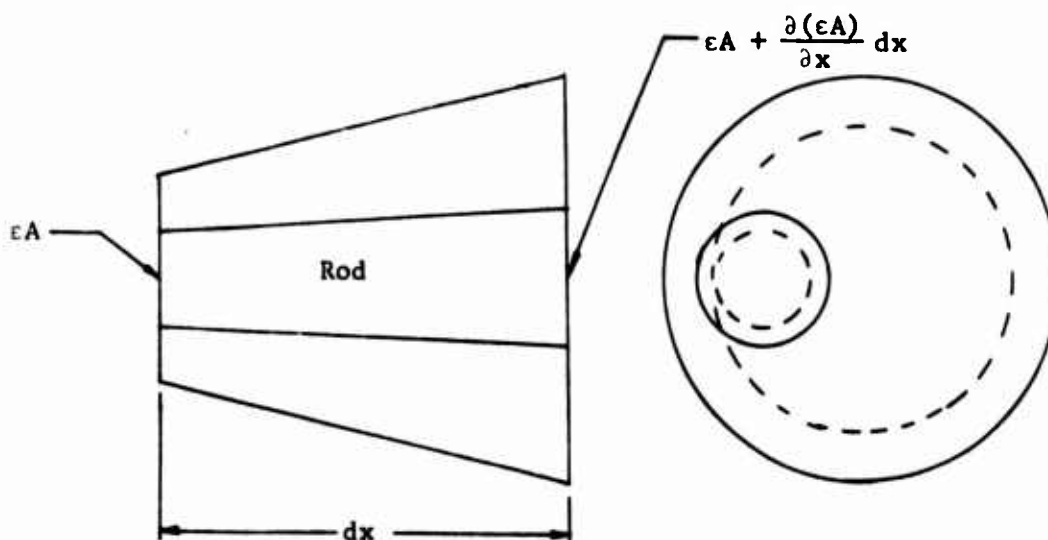


Figure A3 - Particle Rod Model

The net pressure force acting on the "particle rod", p_{nr} , is then

$$p_{nr} = pA\epsilon + \left(p + \frac{\partial p}{\partial x} \frac{dx}{2}\right) \frac{\partial(A\epsilon)}{\partial x} dx - \left(p + \frac{\partial p}{\partial x} dx\right) [A\epsilon + \frac{\partial(A\epsilon)}{\partial x} dx]$$

or neglecting second order terms

$$p_{nr} = - \frac{\partial p}{\partial x} A\epsilon dx$$

Note that the pressure acting on the particle phase in this model acts on an area ϵA , while the pressure acting on the gas phase acts on an area $(1-\epsilon)A$. Thus, for the rod model, the pressure force acting on the particle and gas phases are respectively $-A\epsilon \frac{\partial p}{\partial x}$ and $-A(1-\epsilon) \frac{\partial p}{\partial x}$.

Recognizing that in this model the interaction force does not contain a pressure gradient term (F not \bar{F} must be used) we have consistency between the simple rod model and the complicated continuum model.

3. Energy Equations

Before deriving the energy equations for the gas and particle phases, let us review the general energy equation for a control volume. The first law of thermodynamics for a control volume which is fixed in space (Eulerian approach) is

$$Q_A = P_{\text{shaft}} + P_{\text{shear}} + \int_{\text{c.v.}} \frac{\partial}{\partial t} \left[\rho \left(E + \frac{u^2}{2} \right) \right] dV \\ + \oint_{\text{c.s.}} \left(H + \frac{u^2}{2} \right) \rho u \, dA.$$

where

- Q_A = rate of heat added to the control volume (energy per unit time)
 P_{shaft} = power delivered from medium inside the control volume to the outside, due to rotating mechanical members (work per unit time)
 P_{shear} = power transferred from medium within the control volume to adjacent outside medium through shear force.

Note that the outside medium must be in motion to have power delivered; if the outside medium is stationary, the power will be zero even though there is force transmitted.

$\int_{\text{c.v.}} [] dV$ = the time rate of increase of the internal and kinetic energy of the medium inside the control volume.

$\oint_{\text{c.s.}} [] dA$ = the net enthalpy flux and kinetic energy flux going out of the control surface, (work per unit time).

E = internal energy of gas per unit mass of gas

$H = E + \frac{P}{\rho}$ = enthalpy of gas per unit mass of gas.

The energy equation for the gas phase is then

$$\sigma A(q + q_w) = F u_p A + \phi_I A + \frac{\partial}{\partial t} [\rho(1-\epsilon)A \left(E + \frac{u^2}{2} \right)] + \\ + \frac{\partial}{\partial x} [\rho u(1-\epsilon)A \left(E + \frac{u^2}{2} + \frac{P}{\rho} \right)] \\ - \omega A \left(\hat{E} + \frac{u^2}{2} - \frac{P}{\rho_p} \right) + \omega_w A \left(E_w + \frac{u_w^2}{2} + \frac{v_w^2}{2} + \frac{P_w}{\rho_w} \right) + \omega_{wp} \frac{P}{\rho_p} A \quad (A17)$$

where the total dissipation ϕ has been broken down into a boundary dissipation term ϕ_B , and an internal dissipation term, ϕ_I (see Appendix B) namely:

$$\phi = \phi_I + \phi_B$$

where

$$\phi_B = F_w(u_{wa} - u) - F(u_p - u)$$

The term \hat{E} is the internal energy of the combustion products calculated at the flame temperature and is not included in q . Care must be taken in supplying the value of q to insure that \hat{E} is not included. In writing Eq. (A17), we have assumed that the values of q and \hat{E} do not include the effects of the velocity of the particles and the flow work. Resulting

from the creation of gas mass, thus these terms are treated separately in the 5th term on the right hand side of Eq. (A17). It is felt that the kinetic energy attributed to the velocity of the combustion products as they move away from the surface of the burning propellant is included in q and need not be isolated. The sixth term on the right hand side accounts for the energy lost by gas passing through the wall. The last term represents the flow work associated with particles leaving through the wall.

When calculating the work done on the surroundings, it should be noted that there is no work done by the wall friction force since the wall is stationary; however, the interaction force F (remembering that in accordance with the simplified model the interaction force is F and not \bar{F}) does do work since the gas particle boundary has a velocity equal to u_p . To clarify this point, let us first consider a viscous fluid flowing next to a stationary solid wall (see Fig. (A4)). The velocity of the fluid in contact with the wall must be zero. The velocity increases from zero at the wall, through the boundary layer to its "free stream" value of u . If our control volume is taken with the solid wall as a boundary, then the shear force F_s does no work on the medium outside the control volume, because the boundary of the medium is at zero velocity. The viscous stress in the boundary layer within the control volume will dissipate mechanical energy into heat, but this energy transfer is within the control volume and does not represent energy transfer across the control volume boundary. If the boundary of the control volume is another fluid, then the rate of work

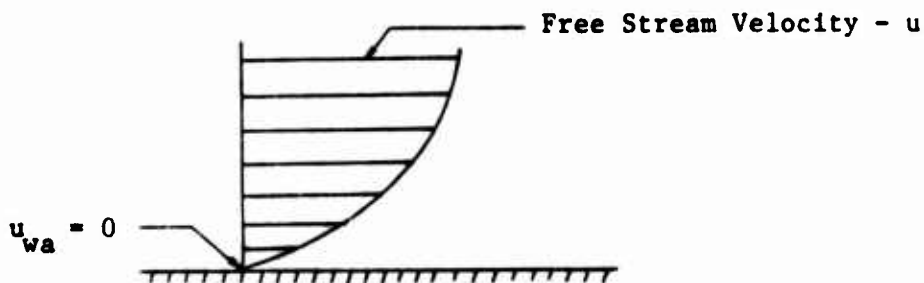


Figure (A4) - Viscous flow next to a wall

done by the medium to the outside, p_{shear} , is $F_S u_b \text{ Adx}$, where u_b is the velocity of the common boundary of the fluids, not their free stream velocities. If the boundary is a solid moving at a velocity u_b , then the rate of work done is also $F_S u_b \text{ Adx}$.

In our present case, the particle phase is "solid", therefore the rate of work done by the gas on the particle is $F u_p \text{ Adx}$ and conversely the rate of work done by the particles on the gas is $-F u_p \text{ Adx}$.

If we now define Q and Q_w as the total energy addition terms due to burning and energy transfer through the wall, respectively, as

$$Q = [q\sigma + \omega(\hat{E} + \frac{1}{2} u_p^2 - \frac{p}{\rho_p})] \quad (\text{A18})$$

and

$$Q_w = [q_w\sigma - \omega_w(E + \frac{1}{2} u_w^2 + \frac{1}{2} v_w^2 + \frac{p_w}{\rho_w})] \quad (\text{A19})$$

and simplify Eq. (A17) by subtracting Eq. (A2) multiplied by $(E + u^2/2)$ and Eq. (A10) multiplied by u , we arrive at the final version of the energy equation for the gas phase, namely:

$$\begin{aligned} \frac{DE}{Dt} + \frac{p}{\rho} \frac{\partial u}{\partial x} - \frac{pu}{\sigma} \frac{\partial \epsilon}{\partial x} = \frac{1}{\sigma} \left[Q + Q_w + u(F - F_w) - F u_p + \phi_I \right. \\ \left. - \omega(u u_p - \frac{1}{2} u^2 + E) + \omega_w(u u_w - \frac{1}{2} u^2 + E) - \omega_{wp} \frac{p}{\rho_p} - \frac{pu(1-\epsilon)}{A} \frac{\partial A}{\partial x} \right] \quad (\text{A20}) \end{aligned}$$

For the current problem, ϕ_I is assumed to be negligible. Similarly, the particle energy equation can be written as

$$\begin{aligned} \sigma_p(q_p + q_{wp})A = -F u_p A + \frac{\partial}{\partial t} [\rho_p \epsilon A (E_p + \frac{1}{2} u_p^2)] + \frac{\partial}{\partial x} [\rho_p \epsilon A u_p (E_p + \frac{1}{2} u_p^2 + \frac{p}{\rho_p})] \\ + \omega(E_p + \frac{1}{2} u_p^2 + \frac{p}{\rho_p})A + \omega_{wp}(E_{wp} + \frac{1}{2} u_{wp}^2 + \frac{1}{2} v_{wp}^2 + \frac{p_w}{\rho_p})A \quad (\text{A21}) \end{aligned}$$

where we have defined the enthalpy of the particle phase, H_p , as

$$H_p = E_p + \frac{p}{\rho_p} \quad (\text{A22})$$

and the enthalpy of the particles leaving through the wall, H_{wp} , as

$$H_{wp} = E_{wp} + \frac{p_w}{\rho_p} \quad (\text{A23})$$

If we now define Q_p and Q_{wp} , the total energy addition terms due to burning and energy transfer with the wall, respectively, as

$$Q_p = [\sigma_p q_p - \omega(E_p + \frac{1}{2} u_p^2 + \frac{p}{\rho_p})] \quad (A24)$$

and

$$Q_{wp} = [\sigma_p q_{wp} - \omega_{wp}(E_{wp} + \frac{1}{2} u_{wp}^2 + \frac{1}{2} v_{wp}^2 + \frac{p_w}{\rho_p})] \quad (A25)$$

and simplify Eq. (A21) utilizing Eqs. (A4) and (A11) we arrive at the final version of the energy equation for the particle phase; namely:

$$\begin{aligned} \frac{D^P E_p}{Dt} + \frac{p}{\rho_p} \frac{\partial u_p}{\partial x} + \frac{p u_p}{\sigma_p} \frac{\partial \epsilon}{\partial x} = \frac{1}{\sigma_p} [Q_p + Q_{wp} \\ + u_p F_{wp} + (E_p + \frac{u_p^2}{2}) (\omega + \omega_{wp}) - \frac{\epsilon p u_p}{A} \frac{\partial A}{\partial x}] \end{aligned} \quad (A26)$$

A simpler form of the particle energy equation, (A26), results if we assume that the pressure term in Eqs. (A22) and (A23) may be dropped and the flow work associated with the particles phase is accounted for by the term $\epsilon A u_p \frac{\partial p}{\partial x}$. This is equivalent to dropping the pressure contribution in the last two terms of Eq. (A21) and replacing the term $\frac{\partial}{\partial x} (\epsilon A u_p p)$ with $\epsilon A u_p \frac{\partial p}{\partial x}$. The resulting particle energy equation is then

$$\frac{D^P E_p}{Dt} = q_p + q_{wp} + \omega_{wp} [(E_p - E_{wp}) - \frac{1}{2} (u_p - u_{wp})^2 + \frac{1}{2} v_{wp}^2] \quad (A27)$$

It should be noted that Eqs. (A26) and (A27) are presented here for the purpose of completeness only. They are uncoupled from the rest of our system and do not enter into the calculations.

Appendix A

REFERENCES

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- A2 Rudinger, G. "Relaxation in Gas-Particle Flow," Chap. 3 in Nonequilibrium Flows Part I, edited by P.P. Wegener, Marcel Dekker, New York, 1969.
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Appendix B*. Derivation of One-Dimensional Tube Flow Equations

During the course of deriving the two-phase flow equations, some basic questions were raised about the approximations involved in the one-dimensional representation of fluid flow in a tube. Most engineering textbooks treat the one-dimensional flow problem by applying the conservation laws to the one-dimensional tube directly, without relating the resulting equations to the three-dimensional field equations. In this appendix, we shall derive the governing equation for one-dimensional, one-phase tube flow, from the general three-dimensional field equations, and indicate the approximations involved.

The three-dimensional governing differential equations are (see, for example, Refs. B1 and B2.)

the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0, \quad (B1)$$

the momentum equation

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + X_i + \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_j} \quad (B2)$$

and the energy equation

$$\frac{DE}{Dt} + \frac{p}{\rho} \frac{\partial u_i}{\partial x_i} = Q + \frac{1}{\rho} \phi - \frac{1}{\rho} \frac{\partial q_i}{\partial x_i} \quad (B3)$$

where X_i is the component of force per unit mass due to external sources, τ_{ij} is the viscous stress tensor, Q is the heat addition per unit mass per unit time, q_i is the heat conduction within the element, and ϕ is the dissipation function given by

$$\phi = \frac{1}{2} \tau_{ij} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (B4)$$

We shall first make the approximation that $u_2 \ll u_1$, $u_3 \ll u_1$ and thus the only non-vanishing component of velocity is u_1 . In a more precise manner, we may relax the requirement on u_2 and u_3 and only require that their integral across the area normal to the flow direction be small, namely:

$$\iint_A \begin{matrix} u_2 \\ u_3 \end{matrix} dA \ll \iint u_1 dA \quad (B5)$$

where for convenience we will interchangeably use the notation (x,y,z) corresponding to (x_1, x_2, x_3) . For simplicity, we shall drop the u_2 and u_3 terms right from the beginning. Equations (B1) to (B3) then reduce to

* Dr. Aivars Celmins first proposed the definitions of average quantities used in this Appendix and the approximations involved.

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \quad (B6)$$

$$\rho \frac{Du}{Dt} + \frac{\partial p}{\partial x} - \rho X - \frac{\partial \tau_{11}}{\partial x_j} = 0 \quad (B7)$$

$$\frac{DE}{Dt} + \frac{p}{\rho} \frac{\partial u}{\partial x} = Q + \frac{1}{\rho} \left[\tau_{xx} \frac{\partial u}{\partial x} + \tau_{xy} \frac{\partial u}{\partial y} + \tau_{xz} \frac{\partial u}{\partial z} \right] - \frac{1}{\rho} \frac{\partial q_1}{\partial x_1} \quad (B8)$$

where the subscript on u has been dropped. Integrating the continuity equation, (B6) over the cross section of the duct, we have

$$\left[\iint_A \left(\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} \right) dA \right] dx = 0 \quad (B9)$$

We may interchange the order of the x differentiation on the area integration without using a double integral extension of Leibnitz's rule, which is not readily available, by considering the area integration as a single integration. Referring to Fig. (B1) it can be shown that if

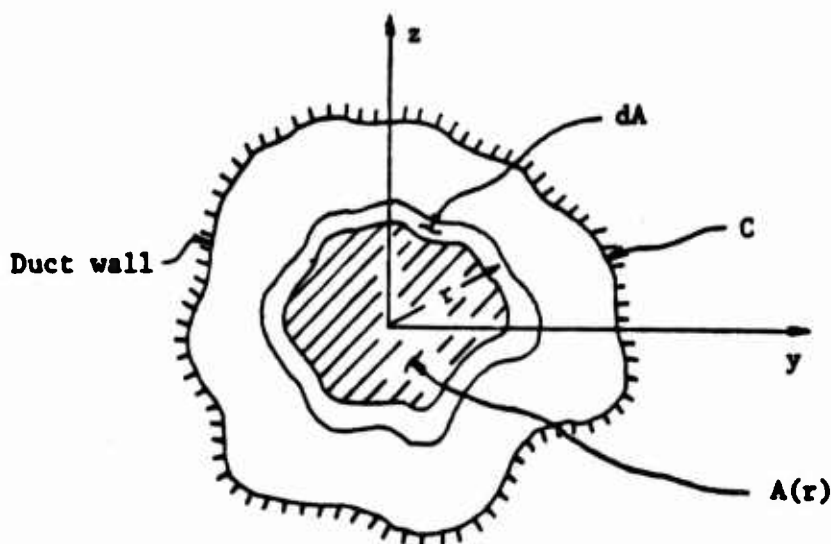


Figure (B1) Diagram Showing Cross Section of the Duct

a parameter $r = r(y, z)$ exists such that

$$\Gamma(x, y, z, t) = \Gamma(x, r, t) \quad (B10)$$

and

$$A = A(r) \quad (B11)$$

where Γ is any flow variable (note that for a circular cross section r is the radius and $A(r) = \pi r^2$)

then

$$\iint_A \frac{\partial}{\partial x} \Gamma \, dA = \frac{\partial}{\partial x} \iint_A \Gamma \, dA - \Gamma|_C \frac{dA}{dx} \quad (B12)$$

where C is the boundary of the cross section of the duct. If Γ vanishes on C, we then have

$$\iint_A \frac{\partial}{\partial x} \Gamma \, dA = \frac{\partial}{\partial x} \iint_A \Gamma \, dA \quad (B13)$$

Applying Eq. (B13) to Eq. (B9), assuming that u vanishes on C, we arrive at the continuity equation in terms of average properties, namely:

$$\frac{\partial}{\partial t} (A\bar{\rho}) + \frac{\partial}{\partial x} (A\bar{\rho} \bar{u}) = 0 \quad (B14)$$

where the average density $\bar{\rho}$ and average velocity \bar{u} are given by

$$\bar{\rho} = \frac{1}{A} \iint_A \rho \, dA \quad (B15)$$

$$\bar{u} = \frac{1}{A\bar{\rho}} \iint_A \rho u \, dA \quad (B16)$$

Note that \bar{u} as defined by Eq. (B16) is the "weighted" average, not the simple average, \bar{u}^* , given by

$$\bar{u}^* = \frac{1}{A} \iint_A u \, dA \quad (B17)$$

The quantity \bar{u}^* does not satisfy the continuity equation exactly.

The momentum equation, (B7), when combined with (B6) multiplied by u , can be written as

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial p}{\partial x} = \rho X + \frac{\partial \tau_{11}}{\partial x_j} \quad (B18)$$

Integrating this equation over the cross section, and applying Eq. (B12), we obtain

$$\begin{aligned} \frac{\partial}{\partial t} \iint_A (\rho u) dA + \frac{\partial}{\partial x} \iint_A \rho u^2 dA + \frac{\partial}{\partial x} \iint_A p dA \\ - p_C \frac{dA}{dx} = \iint_A \rho X dA + \iint_A \frac{\partial \tau_{1j}}{\partial x_j} dA \end{aligned} \quad (B19)$$

The last term in (B19) may be integrated as

$$\begin{aligned} \iint_A \frac{\partial \tau_{1j}}{\partial x_j} dA = \iint_A \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) dy dz \\ = \iint_A \frac{\partial}{\partial x} \tau_{xx} dy dz + \int_C (-\tau_{xz} dy + \tau_{xy} dz) \end{aligned} \quad (B20)$$

where Green's lemma has been used. The last term of (B20) is the axial component of the shear force on the boundary of the cross section, which will be designated as F_w . Defining the averages \bar{p} and \bar{X} by

$$\bar{p} = \frac{1}{A} \iint_A p dA \quad (B21)$$

$$\bar{X} = \frac{1}{A\rho} \iint_A \rho X dA \quad (B22)$$

Eq. (B19) can be written as

$$\begin{aligned} \frac{\partial (A\rho \bar{u})}{\partial t} + \frac{\partial}{\partial x} (A\rho \bar{u}^2) + A \frac{\partial \bar{p}}{\partial x} = A\rho \bar{X} + F_w - \bar{p} \frac{dA}{dx} \\ + p_C \frac{dA}{dx} + \iint_A \frac{\partial}{\partial x} \tau_{xx} dA - \frac{\partial}{\partial x} \iint_A \rho u^2 dA + \frac{\partial}{\partial x} (A\rho \bar{u}^2) \end{aligned} \quad (B23)$$

where the term $\frac{\partial}{\partial x} (A\rho \bar{u}^2)$ has been added to both sides of the equation.

Combining Eq. (B23) with (B14) and neglecting the last five terms in (B23), the one-dimensional momentum equation becomes

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x} = \bar{X} + \frac{F_w}{A\rho} \quad (B24)$$

The approximation involved in deriving the momentum equation is then

$$\left| \iint_A \frac{\partial \tau_{xx}}{\partial x} dA \right| \ll |F_w| \quad (B25)$$

$$\left| \iint_A (\rho u^2) dA - A \bar{\rho} \bar{u}^2 \right| \ll |A \bar{\rho} \bar{u}^2| \quad (B26)$$

$$\left| \frac{dA}{dx} (p_C - \bar{p}) \right| \ll \left| A \frac{\partial \bar{p}}{\partial x} \right| \quad (B27)$$

The term F_w is the frictional force per unit axial length between the fluid and the wall; it may be measured experimentally, or estimated.

The conservation of energy, in differential equation form, after neglecting u_2 and u_3 , is given by Eq. (B8). Adding Eq. (B6) multiplied by E to Eq. (B8) multiplied by ρ and integrating over the cross section, we arrive at

$$\begin{aligned} \iint_A \left[\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho E u)}{\partial x} \right] dA = \iint_A \left(\rho Q - \frac{\partial q_1}{\partial x_1} - \frac{\partial}{\partial x}(\rho u) + u \frac{\partial p}{\partial x} + \tau_{xx} \frac{\partial u}{\partial x} \right. \\ \left. + \tau_{xy} \frac{\partial u}{\partial y} + \tau_{xz} \frac{\partial u}{\partial z} \right) dy dz \quad (B28) \end{aligned}$$

The last three terms in Eq. (B28) represent the viscous dissipation, $\bar{\phi}$. The last two terms will be simplified according to the following:

$$\begin{aligned} & \iint_A \left(\tau_{xy} \frac{\partial u}{\partial y} + \tau_{xz} \frac{\partial u}{\partial z} \right) dy dz \\ &= \iint_A \left[\frac{\partial(\tau_{xy} u)}{\partial y} + \frac{\partial(\tau_{xz} u)}{\partial z} \right] dy dz - \iint_A \left(u \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) dy dz \\ &= \int_C (\tau_{xy} u dz - \tau_{xz} u dy) - \iint_A u \left(\frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) dy dz \\ &= F_w u_w - \iint_A \bar{u} \left(\frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) dy dz + \iint_A (\bar{u} - u) \left(\frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) dy dz \\ &= F_w u_w - F_w \bar{u} + \iint_A (\bar{u} - u) \left(\frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) dA \end{aligned}$$

or

$$\bar{\Phi} = \bar{\Phi}_B + \bar{\Phi}_I \quad (B29)$$

where

$$\bar{\Phi}_B = F_w u_{wa} - F_w \bar{u}$$

$$\bar{\Phi}_I = \iint_A \left[(\bar{u} - u) \left(\frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) + \tau_{xx} \frac{\partial u}{\partial x} \right] dA \quad (B30)$$

and u_{wa} is the velocity of the fluid at the wall. The first term on the right hand side of Eq.(B29), $\bar{\Phi}_B$, represents the dissipation of energy through wall friction (boundary dissipation). The term $\bar{\Phi}_I$ represents internal dissipation. The reason for separating the total viscous dissipation, $\bar{\Phi}$, into these two components is to conform to the accepted engineering practice of utilizing a wall friction coefficient for one-dimensional problems. It must be realized that the application of a steady state friction coefficient to an unsteady problem may involve substantial error.

If we now make the following definition for average quantities,

$$\bar{E} = \frac{1}{A\bar{\rho}} \iint_A \rho E dA \quad (B31)$$

$$\bar{Q} = \frac{1}{A\bar{\rho}} \iint (\rho Q - \frac{\partial q_1}{\partial x_1}) dA \quad (B32)$$

and neglect certain terms, which involve the following approximations,

$$\left| \iint_A \rho E u dA - \bar{\rho} \bar{E} \bar{u} A \right| \ll \left| \bar{\rho} \bar{E} \bar{u} A \right| \quad (B33)$$

$$\left| \iint_A \rho u dA - \bar{\rho} \bar{u} A \right| \ll \left| \bar{\rho} \bar{u} A \right| \quad (B34)$$

$$\left| \iint_A u \frac{\partial p}{\partial x} dA - \bar{u} \frac{\partial \bar{p}}{\partial x} A \right| \ll \left| \bar{u} \frac{\partial \bar{p}}{\partial x} A \right| \quad (B35)$$

Equation (B28) reduces to

$$\frac{\partial (A\bar{\rho} \bar{E})}{\partial t} + \frac{\partial (A\bar{\rho} \bar{E} \bar{u})}{\partial x} = \bar{\rho} A \bar{Q} - A \bar{p} \frac{\partial \bar{u}}{\partial x} + F_w (u_w - \bar{u}) + \bar{\Phi}_I \quad (B36)$$

Combining (B36) with (B14) and, (B24) multiplied by \bar{u} , we obtain,

$$\frac{D}{Dt} \left(\bar{E} + \frac{\bar{u}^2}{2} \right) = - \frac{1}{A\bar{\rho}} \frac{\partial}{\partial x} (A\bar{u} \bar{p}) + \bar{X} \bar{u} + \bar{Q} + F_w u_w / A\bar{\rho} + \frac{\bar{\phi}_I}{A\bar{\rho}} \quad (B37)$$

If the dissipation function $\bar{\phi}$ had not been separated as in Eq.(B29), Equation (B37) would then become

$$\frac{D}{Dt} \left(\bar{E} + \frac{\bar{u}^2}{2} \right) = - \frac{1}{A\bar{\rho}} \frac{\partial}{\partial x} (A\bar{u} \bar{p}) + \bar{X} \bar{u} + \bar{Q} + \frac{F_w}{A\bar{\rho}} \bar{u} + \frac{\bar{\phi}}{A\bar{\rho}} \quad (B38)$$

Under certain situations $\bar{\phi}_I$ in Eq.(B37) may be neglected. It is realized that $\bar{\phi}$ must at all times be positive and if the problem is such that either $\bar{\phi}_B$ or $\bar{\phi}_I$ are negative this assumption must be reexamined. For all practical problems, $(u_w - \bar{u})$ and F_w are opposite in sign, therefore, the term $\bar{\phi}_B$ is positive. Within the boundary layer where $\partial \tau_{xy} / \partial y$ and $\partial \tau_{xz} / \partial z$ are large and positive, the term $(\bar{u} - u)$ is also positive, therefore, $\bar{\phi}_I$ is also positive.

The one-dimensional equations are, in general, good for flows of close to uniform velocity distribution. The viscous force is then negligible except near the solid wall, where a thin layer of boundary conditions exist. This boundary layer is responsible for the wall friction term F_w .

A typical set of one-dimensional tube flow equations may be found in Ref. (B3).

References of Appendix B.

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2. Oswatitsch, Klaus, "Gas Dynamics", English version by G. Kuerti, Academic Press Inc., N.Y. 1956.
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APPENDIX C - COMPUTER CODE

This appendix contains a complete description of the computer code TWOFLO including input and output information. A brief explanation of the function of each subroutine used in the code is presented along with instructions for altering the user specified routines. The nomenclature used in the actual code is, wherever possible, consistent with this report limited only by the fact that Greek symbols and lower case letters are not available in Fortran IV the code language. TWOFLO is written to accept any consistent set of units or can be run nondimensionally.

1. Description of Fortran Variables

The following is a list of the major FORTRAN variables used in the TWOFLO code. Those variables followed by a dash, e.g. UP-, are suffixed with several different qualifying symbols, point numbers, point letters, variables of differentiation, and so forth. For an explanation of these symbols, see 3 below.

1. Flow variables

CG-	=	c
EG-	=	E
EP-	=	E _p
ES-	=	E
PG-	=	p
RG-	=	ρ
RP-	=	ρ _p
TG-	=	T
UG-	=	u
UP-	=	u _p
XX-	=	x

2. Miscellaneous variables

GC-	=	GC
GM-	=	GM
GE-	=	GE
PC-	=	PC
PM-	=	PM
PE-	=	PE
F-	=	F
FWG-	=	F _w
FWP-	=	F _{wp}
QG-	=	Q
QP-	=	Q _p
QWG-	=	Q _w
QWP-	=	Q _{wp}
W-	=	ω
WWG-	=	ω _w
WWP-	=	ω _{wp}

DTT- = Δt
 Dt- = Δt
 DX- = Δx

3. Suffixes - suffixes are used to describe

a. mesh points, i.e. SP(K,I) where

K = time line (1,2)

I = point number

b. a particular point in the iteration scheme i.e. SP1, SPA, etc. where 1 and A are point designations.

c. derivatives, i.e. SPX-, SPT- and GEUG-

SPX- = $\partial \sigma_p / \partial x$

SPT- = $\partial \sigma_p / \partial t$

GESp- = $\partial GE / \partial \sigma_p$

(suffixes X and T represent x and t respectively)

II. Description of subroutines *

1. ABC(L,K1,K2,K3,I1,I2,I3,M1,M2,M3,J2,IC,ID,NNW1,NNW2,TT1,TT2,TT3,TTT,NXT)

This subroutine is designed to interpolate for the properties at the base of the characteristics when only the gas phase is present. When quadratic interpolation is required, a Lagrange interpolating polynomial of order two is used: namely

$$y(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} y_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} y_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} y_3$$

where $y(x)$ is the particular property to be calculated, and y_1 , y_2 and y_3 are the values of that property at the mesh points.

The terms in the call list are

K1	=	1	calculate properties at points A,B and C
	=	2	" " " point A
	=	3	" " " " B
	=	4	" " " points A and C
	=	5	" " " " B and C
	=	6	" " " point C

* Note: For all subroutines, L = 1 indicates that the point is located behind the bullet; L = 2 indicates that point is located in front of the bullet.

K2 = 1 C properties are assigned to be the same as point (M1,IC)
 K2 \neq 1 C properties are interpolated
 K3 = 1 C properties are not calculated (used after first
 iteration when K2 = 1)

I1,I2,I3 = point numbers

M1,M2,M3 = line number of points I1,I2,I3 respectively. (1 old time
 line--- 2 new time line)

J2 = 1 quadratic interpolation is used between points I1,I2 and I3

J2 = 2 linear interpolation is used between points I1 and I2.

IC = (K2=1) IC is the point number of the mesh point correspond-
 ing to point C.

ID = not used

NNW1 = " "

NNW2 = " "

TT1,TT2,TT3 = times associated with points I1,I2, and I3 respectively
 if interpolation is with respect to time instead of
 position.

TTT = not used

NXT = 1 interpolation along a constant time line using
 position

= 2 interpolation using time

2. ABCD(L,K1,K2,K3,I1,I2,I3,M1,M2,M3,J2,IC,ID,NNW1,NNW2,
 TT1,TT2,TT3,TTT,NXT)

This subroutine is quite similar to ABC except here the
 properties of both phases are calculated. The terms in the call list
 which are different from ABC are

K1 = 1 calculate properties at points A,B,C and D

= 2 " " " " A,C and D

= 3 " " " " B,C and D

= 4 " " " point A

= 5 " " " B

= 6 " " " B

= 7 " " " D

= 8 " " " C

= 9 " " " C

20 do no calculating just print A,B,C and D properties

K2 = 1,4,5 properties at point C correspond to properties at
 point (M1,IC)

2,3 properties at point D correspond to properties at
 point (M1,ID)

ID = the point number of the mesh point corresponding to
 point D if K2 = 2 or 3.

3. ADISC(L,ID,K1,K2,K3,K4,K5)

This routine has two purposes: it handles discontinuities in
 cross-sectional area, $A(x)$, and is used also, either in conjunction
 with INRTBN or simply by itself, to handle the gas-particle interface,
 when that interface is treated as a discontinuity in gas concentration
 (σ). Both of these purposes are accomplished with much the same

computational procedure. There are two main differences, however. The first is that, in the case of the gas-particle interface, no particle properties are calculated in front of the discontinuity, since no particles are present there; the second is that, in the case of the gas-particle interface, the u-c characteristic may intersect with the path of the bullet, and if it does, the properties at the base of that characteristic must be obtained by interpolation along the bullet path.

The terms in the call list are:

ID = point number of the point on the left hand side of the area discontinuity

K1 = 0 normal Area Discontinuity

= 1 Gas-particle interface

K2 = not used

K3 = " "

K4 = " "

K5 = " "

4. ADT(C1,C2,C3,U1,U2,U3,X1,X2,X3,UP1,UP2,UP3,K1,K2,KK3)

This subroutine calculates the Δt associated with each point.

The derivation is as follows:

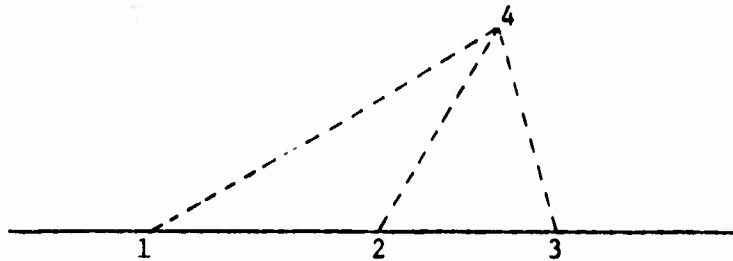


Figure B1. Plot of characteristic grid used to calculate Δt .

Referring to Fig.(B1), we first calculate Δt (DT1) associated with the (u+c) characteristic direction by writing

$$\frac{x_4 - x_1}{DT1} = \frac{(u_4 + c_4) + (u_1 + c_1)}{2}$$

$$\frac{x_4 - x_2}{DT1} = \frac{u_4 + u_2}{2}$$

Rewritten, these equations are

$$x_4 = x_1 + DT1 \cdot \frac{1}{2} (u_4 + c_4 + u_1 + c_1)$$

$$x_4 = x_2 + DT1 \cdot \frac{1}{2} (u_4 + u_2)$$

Subtracting these two equations, we obtain

$$0 = (x_1 - x_2) + DT1 \cdot \frac{1}{2} (c_4 + c_1 + u_1 - u_2)$$

If we now assume that $c_4 = c_2$, we have

$$DT1 = \frac{2(x_2 - x_1)}{c_2 + c_1 + u_1 - u_2}$$

A similar argument leads to $\Delta t(DT3)$ associated with the (u-c) characteristic, namely:

$$DT3 = \frac{2(x_2 - x_3)}{u_3 - u_2 - c_2 - c_3}$$

The terms in the call list are

C1,C2,C3, = CG at points 1,2 and 3 respectively
 U1,U2,U3 = UG " "
 X1,X2,X3 = XX " "
 UP1,UP2,UP3 = UP

K1 = 1 interior point
 2 interface between gas and two-phase region
 3 area discontinuity
 K2 = 1 smallest value of Δt resulting from u+c and u-c
 is chosen
 2 Δt resulting from u+c is chosen
 3 " " u-c " "

KK3 = not used.

5. AIN(IFILE,IA,KK1,KK2,KK3,KK4)

This subroutine is used to read in data from a dump tape.

The terms in the call list are

IFILE = number of the file from which data is read.

IA = data is assigned to mesh point (IA,).

KK1 = not used

2 = " "

3 = " "

4 = " "

6. AOUT(IFILE,IA,KK1,KK2,KK3,KK4)

This subroutine is the same as AIN except that it dumps data on
 IFILE

7. AR(XX,Z1,Z2) USER SPECIFIED

This function subroutine calculates the cross-sectional area of the duct, A, given the x location.

8. ARX(XX,Z1,Z2) USER SPECIFIED

This function subroutine calculates $\partial A / \partial x$ given x.

9. BNPTG(L,I1,I2,I3,MAXIT,J1,J2,J3,J4)

This subroutine calculates the gas phase properties at boundary points using one phase equations

The terms in the call list are:

I1,I2,I3 = base mesh points (point being calculated is I1
if J1 = 1 or I3 if J1 = 2)
MAXIT = maximum number of iterations
J1 = 1 left boundary
2 right boundary
J2 = 1 specify velocity on the boundary
2 " pressure
J3 = 1 normal boundary
= 2,3,4 special boundary points
J4 = 1 J2=1 the bullet momentum equation is used
2 J2=1 the velocity (bullet) is zero.
3 boundary conditions are determined prior to
entering BNPTG(not in GBCOND)

10. BNSH(L,K1,J4,MAXIT,JJ1,JJ2,JJ3)

This subroutine controls the calculation of a shock reflecting from a boundary

The terms in the call list are

K1 = shock number
J4 = 1 bullet is moving
2 bullet is stationary
MAXIT = maximum number of iterations
JJ1 = not used
JJ2 = " "
JJ3 = " "

11. COMEQ1(L,M,K1,K2,K3,Z1,Z2,Z3)

Using the compatibility equation along the characteristic direction $dx/dt = u_p$, Eq.(50), this routine solves for u_p at point 4, given values of the other material properties.

The terms in the call list are:

```
M = 1
K1 = 1
Z1 =      not used
Z2 =      "   "
Z3 =      "   "
```

12. COMEQ2(L,M,K1,K2,K3,Z1,Z2,Z3)

This subroutine uses the particle energy equation, Eq.(52) written in finite-difference form to solve for E_p at point 4, given values of the other material properties.

Note: This routine is not used, because the particle energy equation is uncoupled from the rest of the system.

13. COMEQ3(L,M,K1,K2,K3,N2,Z2,Z3)

This subprogram calculates σ_p at point 4 given values of the other material properties at point 4. The particle continuity equation Eq.(51), written in finite-difference form, is used.

The terms in the call list are:

```
M = 1
K1 = 1
K2 = not used
K3 = J2 in GNPT
N2 = number of point being calculated (point 4)
Z1 = not used
Z2 = "   "
```

14. COMEQ4(L,M,K1,K2,K3,Z1,Z2,Z3)

This routine uses the compatibility equation along the direction $dx/dt = u$, Eq.(47).

The terms in the call list are:

```
M = 1      two phase compatability equations is used
      2,3   gas phase      "      "      "
K1 = 1      equation (47) is solved for EG4
      2      "      (47) "      "      "
           and  $[\partial E / \partial \sigma]_4$  and  $[\partial E / \partial u]_4$  (see NEWTON)
```

K2 =	not used
K3 = 1	PM4, PC4, GC4, GE4 are recalculated
2	" " " " are not recalculated
Z1 =	not used
Z2 =	" "
Z3 =	" "

15. COMEQ5(L,M,K1,K2,K3,Z1,Z2,Z3)

This subroutine solves the compatibility equation along the direction $dx/dt = u + c$, Eq.(48).

The terms in the call list are:

M = 1,3	two phase compatability equation is used
M = 2	gas " " " "
K1 = 1	equation is solved for either SG4 or UG4 (see K2)
2	equation is put into the form $g(\sigma, u) = 0$ and the derivatives $\partial g / \partial \sigma$ and $\partial g / \partial u$ are calculated (see NEWTON)
K2 = 1	solve for SG4(M=1,3) or RG4(M=2)
2	solve for UG4
K3 =	S.A. COMEQ4
Z1 =	not used
Z2 =	" "
Z3 =	" "

16. COMEQ6(L,M,K1,K2,K3,Z1,Z2,Z3)

This subroutine solves the compatibility equation along the direction $dx/dt = u - c$, Eq.(49).

The terms in the call list are:

M = 1,2	two phase compatability equation is used
= 3	gas phase " " " "
K1 = 1	equation is solved for either SG4, RG4 or UG4 (see K2)
2	equation is put in the form $f(\sigma, u) = 0$ and the derivatives $\partial f / \partial \sigma$ and $\partial f / \partial u$ are calculated.
K2 = 1	solve for SG4(M=1,2) or RG4(M=3)
2	solve for UG4
K3 =	S.A. COMEQ4
Z1 =	not used
Z2 =	" "
Z3 =	" "

17. COMEQ7(L,M,K1,K2,Z1,Z2,Z3)

This routine calculates the regression distance (Z).

L is the only term in the call list that is used

18. COMEQ8(L,M,K1,K2,K3,Z1,Z2,Z3)

This subroutine calculates field properties when UG4 and UP4 are zero and all base point properties are identical.

L is the only term in the call list that is used.

19. CSQ(L,M,K1,K2,RH,E,C,P,PE,PR,T,XA,XB)

This subroutine calculates the sound speed of the gas

The terms in the call list are:

M = 1	RH and E must be input
M = 2	P, RH, PE, PR must be input
K1 =	not used
K2 =	" "
RH =	ρ
E =	E
C =	c
P =	p
PE =	$\partial p / \partial E$
PR =	$\partial p / \partial \rho$
T =	T
XA =	not used
XB =	" "

20. DIFF(L,N,M,K2,K3,Z1,Z2,Z3)

This subroutine uses forward, backward and central difference schemes to calculate the terms $\partial u_p / \partial x$ and $\partial \sigma_p / \partial x$. Then the particle continuity and momentum equations are used to calculate the terms $\partial \sigma_p / \partial t$ and $\partial u_p / \partial t$ respectively.

The terms in the call list are:

N =	point number
M =	line number
K2 = 1	central difference is used
= 2	backward difference is used
= 3	forward " " "
= 4	x derivatives are calculated externally thus only t derivatives are calculated.
K3 =	M
Z1 =	not used
Z2 =	not used
Z3 =	not used

21. DIMEN(L,K1,K2,K3,K4,K5)

This subroutine nondimensionalizes all variables used in the program using B(1,20), B(1,21), B(1,22) as nondimensionalizing factors.

The terms in the call are:

K1 = 1 nondimensionalize B properties
 2 nondimensionalize points K4 to K5 on the K3
 time line.
 3 dimensionalize

K2 = not used
K3 = time line number
K4 = first point to be treated
K5 = last " " " "

22. DROP(IDR)

This subroutine drops the IDR point from the 1 time line

23. DRVX(L,N1,N2,N3,K1,K2,K3,Z1,Z2,Z3)

This subroutine contains both 2 and 3 point forward and backward and central difference schemes.

The terms in the call list are:

N1,N2,N3 = points to be used in differencing scheme

K1 = 1 calculates derivatives of σ_p
 2 " " " up
K2 = 1 forward difference
 2 central "
 3 backward "

K3 = line number

Z1 = not used
Z2 = " "
Z3 = " "

24. DTQ(L,ID1,ID2,ID3,DTT)

This subroutine calculates Δt for each point on the time line. The smallest value after being reduced by a factor (0.9) becomes the Δt for the next time line calculation

The terms in the call list are:

ID1 = not used
ID2 = " "
ID3 = " "
DTT = Δt

25. DZDT(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,Z1,Z2,L) USER SPECIFIED

This function subroutine is used to calculate the regression rate, D^PZ/Dt .

The only requirement in the call list is that the variables used in the equation for the regression rate be available.

26. ERH(L,IQ,EI,PI,RHI,PMEES,PMRS,XA,TI)

This subroutine uses the equation of state to calculate ρ or E. The Newton Raphson technique is used except for an Ideal gas.

The terms in the call list are:

IQ = 1 calculate ρ given E and p
2 " " E " ρ " p

EI = E

PI = p

RHI = ρ

PMEES = $\partial p / \partial E$

PMRS = $\partial p / \partial \rho$

XA = not used

TI = T

27. FQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,Z1,Z2,L) USER SPECIFIED

This subroutine calculates the drag force, F, between the particles and the gas.

The only requirement in the call list is that the variables used in the equation for the drag force be available.

28. FRET(L,K1,K2,FRW,FTW,FEW,TW,RW,EW,XA,XB) USER SPECIFIED

This subroutine computes the derivatives of $f(\rho, E, T)$ with respect to ρ , E and T.

The terms in the call list are:

K1 = not used

K2 = 1 Virial equation of state.

= 2 Van der Waal equation of state.

K3 = not used

FRW = $\partial f / \partial \rho$

FTW = $\partial f / \partial T$

FEW = $\partial f / \partial E$

TW = T

RW = ρ

EW = E

XA = not used

XB = not used

29. FWGQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT
K1,K2,K3,Z1,Z2,L) USER SPECIFIED

This subroutine calculates the wall friction force acting on the gas, F_{wg} .

The only requirement in the call list other than K1 is that the variables used in the equation for the wall friction force, F_{wg} , be available.

- K1 = 1 calculate F_{wg}
- = 2 calculate F_{wg} , $\partial F_{wg}/\partial u$ and $\partial F_{wg}/\partial p$

30. FWPQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT
K1,K2,K3,Z1,Z2,L) USER SPECIFIED

This subroutine is the same as FWGQ except that it calculates the wall friction force acting on the particles, F_{wp} .

31. GBCOND(L,M1,M2,K3,K4,XA,XB,PGG,UGG)

The subroutine is used to supply gas boundary conditions.

The terms in the call list are:

- M1 = 1 left boundary
- 2 right boundary
- M2 = 1 velocity is specified on the boundary
- 2 pressure " " " " "
- K3 = point number of the boundary point
- K4 = 2 bullet has not moved and $u = 0$.
- XA = not used
- XB = not used
- PGG = pressure
- UGG = velocity

32. GC(SG,SP,UG,UP,EG,EP,RG,RP,CG,PG,PP,TG,TP,ES,F,FWG,FWP
W,WWG,WWP,QG,QP,QWG,QWP,AR,ARX,Z1,Z2,L)

This subroutine calculates the right hand side of the gas continuity equation, GC.

The only requirement in the call list other than Z1 is that the variables used in the equation for GC be available. (the variables F,FWG -----QWP are values generated by subroutines FQ,FWGQ-----QWPQ respectively and AR and ARX are A and $\partial A/\partial x$ respectively)

- Z1 = 1 calculate GC
- = 2 " GC, $\partial GC/\partial u$ and $\partial GC/\partial \sigma$

33. GE(SG,SP,UG,UP,EG,EP,RG,RP,CG,PG,PP,TG,TP,ES,F,FWG,FWP
W,WWG,WWP,QG,QP,QWG,QWP,AR,ARX,Z1,Z2,L)

This subroutine is the same as GC except that the right hand side of the gas energy equation, GE, is calculated.

34. GM(SG,SP,UG,UP,EG,EP,RG,RP,CG,PG,PP,TG,TP,ES,F,FWG,FWP,
W,WWG,WWP,QG,QP,QWG,QWP,AR,ARX,Z1,Z2,L)

This subroutine is the same as GC except that the right hand side of the gas momentum equation, GM, is calculated.

35. GNPT(L,I1,I2,I3,MAXIT,J1,J2,J3,J4)

This subroutine calculates the properties of mesh points in the two-phase region.

The terms in the call list are:

I1,I2,I3 = point numbers

MAXIT = maximum number of iterations

J1 = 1 base properties at points A,B,C and D are calculated internally.

= 2 base properties at points A,C and D are calculated internally. The B properties are calculated externally.

= 3 base properties at points B,C and D are calculated internally. The A properties are calculated externally.

= 4 base properties at points A,B,C and D are calculated externally.

J2 = 1 normal (interior) point is calculated.

= 2 point 4 is located using u_p . The gas compatibility equation is used along $dx/dt = u + c$.

= 3 point 4 is located using u_p . The gas compatibility equation is used along $dx/dt = u - c$.

= 4 two phase left boundary is calculated.

= 5 two phase right boundary is calculated.

= 6 point in front of right traveling shock is calculated.

= 7 point in front of left traveling shock is calculated.

J3 = 1 normal general point

2 initial calculation where interface and bullet boundary are calculated simultaneously.

= 3 area discontinuity point.

J4 = not used.

36. GNPTG(L,I1,K2,K3,MAXIT,J1,J2,J3,J4)

This subroutine calculates the properties of mesh points in the gas only region.

The terms in the call list are:

I1,I2,I3 = point numbers
MAXIT = maximum number of iterations
J1 = not used
J2 = 1 normal (interior) point is calculated.
 = 2,3,4,5 not used
 = 6 point in front of right traveling shock is
 calculated.
 = 7 point in front of left traveling shock is
 calculated.
J3 = not used
J4 = " "

37. GUESS(L,K1,I2,J2,J3,M,JJ5,JJ6)

This subroutine supplies the first guess for the iterations in BNPTG,GNPT and GNPTG.

The terms in the call list are:

K1 = 1 first guess for BNPTG and GNPTG
 = 2 " " " GNPT
I2 = point number of properties used as a
 first guess.
J2 = 1,3 (K1=2) first guess is the point (M,I2)
 2,4 10 (K1=2) first guess is solution of
 linearized two phase equations
 = 6,7 (K1=1) first guess is the point (M,I2)
 = 1,2,3,4, (K1=1) first guess is a solution of
 5,8,9,10 linearized gas phase equations.
J3 = not used
M = line number of properties used as a
 first guess.
JJ5 = not used.
JJ6 = not used.

38. INDISC(L,ID)

This subroutine calculates the complicated singularity that occurs when an area discontinuity exists at the initial bullet location.

The terms in the call list are:

ID = point number of the left point at the area discontinuity.

39. INIT(L,IP,XB,XC,XD)

This subroutine reads in and prints out all initial data.

The terms in the call list are:

```

IP = 0   read in and print out initial data
    = 1   only print out B(      ) array.
    = 2   only print out initial time line
XB =     not used
XC =     "    "
XD =     "    "

```

40. INRTBN(L,M,K1,K2,K3,I1,I2,I3,J1,J2,J3,MAXIT)

This subroutine calculates the gas-particle interface and the bullet boundary simultaneously. It is used until a mesh point is inserted between the two.

None of the terms in the call list are currently used.

41. INTPRN(L,TU,TL,TP,ZZ1,ZZ2,ZZ3,ZZ4)

This subroutine interpolates for and prints out the properties at a time line lying between two calculated time lines.

The terms in the call list are:

```

TU = time of upper time line
TL = " " lower " "
TP = " " interpolated time line
ZZ1 = not used
ZZ2 = " "
ZZ3 = " "
ZZ4 = " "

```

42. INTSEC(X1,U1,C1,T1,X2,U2,C2,T2,X4,U4,C4,T4,N,XB,UB,CB,TB)

This subroutine calculates the x and t location of the point of intersection B, of the line connecting points 1 and 2 and a characteristic emanating from point 4.

The terms in the call list are:

```

X_ = x location of point _
U_ = gas velocity of point_
C_ = sound speed of point_
T_ = time of point_

N = 1 characteristic emanating from point 4 is dx/dt = u + c
    2 " " " " " " dx/dt = u - c
    3 " " " " " " dx/dt = u(u>0)
    4 " " " " " " dx/dt = u(u<0)

```

43. LIMPNO(Y)

This subroutine drops mesh points, one-by-one, until the number of points remaining is equal to MAXPT or MAXPTB. Each mesh point dropped by LIMPNO lies in the region of smallest change in "Y" (with respect to x) where Y is specified in the call statement and can be any one of the flow variables. This helps to insure that a comparatively fine mesh exists in regions of large change, and that a somewhat larger mesh exists in regions of small change.

44. LINAB(L,K1,K2,K3,I1,I2,J1,J2,XP,TP)

This subroutine uses linear interpolation to calculate gas properties at points A or B.

The terms in the call list are:

K1 = 1 calculate A properties
 2 " B "
K2 = 1 input coordinates of end points (I1,J1) and (I2,J2)
 2 input end point properties through common
 blocks LIN1,LIN2,LIN3
K3 = 1 interpolate using position, x.
 2 " " time, t.
I1,I2 = line numbers
J1,J2 = point numbers
XP = x location of point A or B
TP = time of point A or B

45. LOCABC(K1,I1,I2,I3)

This subroutine calculates the x location of points A,B,C and D.

The terms in the call list are:

K1 = 1 point C corresponds to point (1,I2)
 2 " D " " "
I1 = not used
I2 = point number
I3 = not used

46. NEWTON (L,M,K1,K2,K3,K4,Z1,Z2,Z3,Z4)

This subroutine uses Newton Raphson techniques to solve compatibility equations along characteristics $dx/dt = u$, $u + c$

The terms in the call list are:

M = 1	two phase compatibility equations are used
= 2	gas " " equation is used alone
	(dx/dt = u + c
3	" " " " is used alone
	(dx/dt = u - c

K1 = not used

K2 = not used

K3 = 1 GC,GM,GE,PC and PM are held constant during iteration
2 GC,GM,GE,PC and PM vary during iteration

K4 = J2 in GNPT-used to determine the type of point being calculated

Z1 = not used

22 " "

23 - " "

24 - " "

47. NTROPY (L,IQ,RG,EG,SS,JJ1,JJ2,JJ3) USER SPECIFIED

This subroutine is user specified. It's function is to calculate either the entropy, SS, density, RG, or specific internal energy, EG of the gas phase given the other two.

The terms in the call list are:

```

IQ = 1 calculate entropy
    = 2      "      density
    = 3      "      specific internal energy

```

SS = entropy

JJ1 = not used

JJ2 - " "

JJ3 - " "

48. PC(SG,SP,UG,UP,EG,EP,RG,RP,CG,PG,PP,TG,TP,ES,F,FWG,FWP,
W,WWG,WWP,QG,QP,QWG,QWP,AR,ARX,Z1,Z2,L)

This subroutine calculates the right hand side of the particle continuity equation, PC.

The only requirement on the terms in the call list is that all variables used in PC be available.

49. PDV(NLINE,K1,P4,PA,PB,PDXA,PD,XB,PDTA,PDTB)

This subroutine calculates $\sigma_{p,x}$, $\sigma_{p,z}$, $u_{p,x}$ or $u_{p,t}$ at point 4. P4, PA and PB are the values at points 4, A and B of the variable to be differentiated. PDXA PDXB PDTA and PDTB are the values of the derivatives of the said variable at Points A and B.

The terms in the call list are:

NLINE = not used

K1 = 1 calculate x derivatives

 = 2 " t "

50. PE(SG,SP,UG,UP,EG,EP,RG,RP,CG,PG,PP,TG,TP,ES,F,FWG,FWP,
W,WWG,WWP,QG,QP,QWG,QWP,AR,ARX,Z1,Z2,L)

This subroutine calculates the right hand side of the particle energy equation, PE.

The only requirement on the terms in the call list is that all variables used in PE be available.

51. PLOTTO(IT)

This subroutine is used for plotting purposes only.

52. PM(SG,SP,UG,UP,EG,EP,RG,RP,CG,PG,PP,TG,TP,ES,F,FWG,FWP,
W,WWG,WWP,QG,QP,QWG,QWP,AR,ARX,Z1,Z2,L)

This subroutine calculates the right hand side of the particle momentum equation, PM.

The only requirement on the terms in the call list is that all variables used in PM be available.

53. PPLOT(X,Y,NP,NPLOT)

This subroutine is used for plotting purposes only.

54. PRINTO(L,K1,K2,K3,K4,K5,KK6,KK7,KK8,KK9,KK10)

This subroutine controls the printout of calculated data.

The terms in the call list are:

K1 = number of first point to be printed

K2 = " " last " " "

K3 = increment by which points are printed (usually 1)

K4 = number of line to be printed (either 1 or 2)

K5 = 1 print gas properties only

 = 2 print two phase properties

KK6 = not used

KK7 = " "

KK8 = " "

KK9 = " "

KK10 = " "

55. PTARNG(MSR,L)

The subroutine controls the adding and dropping of points to maintain a specified time increment.

The terms in the call list are:

MSR = 1 always

56. PTQ(L,K1,K2,K3,RT,TT,PT,PTT,PTR,XA,XB) USFR SPECIFIED

This subroutine calculates p , $\partial p / \partial T$ and $\partial p / \partial \rho$

The terms in the call list are:

K1 = not used

K2 = 1 Virial equation of state
2 Van der Waals equation of state
3 Ideal gas " " "

K3 = not used

RT = ρ

TT = T

PT = p

PTT = $\partial p / \partial T$

PTR = $\partial p / \partial \rho$

XA = not used

Xb = not used

57. QET(L,K1,K2,RT,TT,ET,XA,XB,XC) USER SPECIFIED

This subroutine uses the equation $f(\rho, E, T) = 0$ to calculate T given ρ and E or to calculate E given ρ and T

The terms in the call list are:

K1 = 1 calculate T
2 " ρ

K2 = 1 Virial equation of state is used
2 Van der Waals equation of state is used

RT = ρ

TT = T

ET = E

XA = not used

XB = " "

XC = " "

58. QGQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DB,TT,K1,K2,K3,Z,L)

This subroutine calculates the rate at which total energy is released during burning of the propellant Q.

The only requirement on the terms in the call list is that all variables used in Q be available.

59. QPQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,ZZ,Z2,L)

This subroutine calculates the rate at which the particles lose energy during burning Q_p .

The only requirement on the terms in the call list is that all variables used in Q_p be available.

60. QUAD(Y1,Y2,Y3,XP)

This subroutine uses quadratic interpolations to calculate the Y property at location XP given Y at points XX1,XX2 and XX3 (i.e., Y1,Y2,Y3 respectively)

61. QWGQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,CG,Z3,CG,Z2,L)

This subroutine calculates the total energy lost by the gas phase due to gas passing through the wall, Q_w .

The only requirements on the terms in the call list is that all variables used in Q_w be available.

62. QWPQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,Z1,Z2,L)

The subroutine calculates the total energy lost by the particle phase due to particles passing through the wall, Q_{wp} .

The only requirements on the terms in the call list is that all variables used in Q_{wp} be available.

63. RHSGAS(L,K1,K2,RG,EG,PG,TG,CG,UG,XX,TT,DT,XA,XB,R1,
R2,R3)

This subroutine calculates the right hand side of the gas continuity (R1), momentum (R2) and energy (R3), and their derivatives with respect to ρ and u .

The only requirement on the terms in the call list other than the variables used in R1, R2 and R3

K1 = 1 calculate R1,R2, and R3
2 " " " " , R3 and their derivatives.

64. SHKFRT(L,K1,K2,KK3,MAXIT,JJ1,JJ2,JJ3)

This subroutine controls the calculation of properties in front of and behind a shock wave.

The terms in the call list are:

K1 = number of the shock
 K2 = 0 normal shock front
 = 1 SHKFRT called from BNSH with special treatment of
 A and B properties
 = 2 not used
 = 3 SHKFRT called from BNSH for initial first guess
 KK3 = not used
 MAXIT = maximum number of iterations
 JJ1 = not used
 JJ2 = " "
 JJ3 = " "

65. SHKIN(L,NR1L2,N2,M2,W,X,Y,Z)

This subroutine controls the initiation of a shock wave.

The terms in the call list are:

NR1L2 = 1 right traveling shock wave
 = 2 left " " "
 N2 = the point number of the point behind the
 inserted shock wave
 M2 = the point number of the first mesh point
 in front of the shock.
 W = not used
 X = " "
 Y = " "
 Z = " "

66. SHKINT(L,K1,MAXIT,KK1,KK2,KK3,KK4)

This subroutine controls the calculation of a shock wave interacting with a gas-particle interface.

The terms in the call list are:

K1 = number of the shock wave
 MAXIT = maximum number of iterations

67. SHOKEQ(L,MS,MQ)

This subroutine solves the Rankin-Hugoniot shock relations for the properties behind a shock wave given either u, p or the shock velocity, U.

The terms in the call list are:

MS = 1 right traveling shock
 2 left " "
 MQ = 1 specify p behind the shock
 2 " u " "
 3 " the shock velocity, U.

68. SHTR(L,J,MM,I)

This subroutine controls the calculation of properties across a shock (currently not in use)

The terms in the call list are:

- J = shock number
- MM = 1 right traveling shock
2 left " "
- I = point number behind the shock

69. SMQ(L,ISM,RW,EW,PW,PRW,PEW,NA,NB,XA,AB,TW)

This subroutine calculates the pressure PW, temperature TW and the derivatives of pressure with respect to density, RW and energy, EW, given density and energy.

The terms in the call list are:

- ISM = 1 calculate p
- 2 calculate p and $\partial p / \partial \rho$
- 3 calculate p, $\partial p / \partial \rho$ and $\partial p / \partial E$
- 4 calculate p and $\partial p / \partial E$

70. SPPT(L,KK1,K2,KK3,PG,TG,EG,XX1,XX2,XX3) USER SPECIFIED

This subroutine calculates C_v, C_p and γ

The terms in the call list are:

- KK1 = not used
- K2 = 1 Virial equation of state is used
- 2 Van der Waal equation of state is used
- 3 Ideal gas equation of state is used

71. SUPINF(Y,YAV,MAXY,MINY,K)

This subroutine determines the maximum MAXY, minimum MINY, and average, YAV values of a variable Y in the call list, and calculates the average change in Y between adjacent mesh points on a given time line.

The terms in the call list are:

- K = 1 behind bullet
- 2 in front of bullet

72. TBCOND(L,K1,K2,K3,K4,XA,XB,UG)

This subroutine specifies the boundary conditions for the gas phase when both phases are present at the boundary.

The terms in the call list are:

K1 = 1 left boundary
 2 right "
K2 = not used
K3 = " "
K4 = " "
XA = " "
XB = " "

73. WQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,ZZ,Z2,L)

This subroutine calculates the rate at which gas mass is created per unit volume of mixture during burning, ω .

The only requirement on the terms in the call list is that all variables used in ω be available.

74. WWGQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,Z1,Z2,L)

This subroutine calculates the rate of decrease in gas mass per unit volume of mixture due to losses through the duct wall, ω_w .

The only requirement on the terms in the call list is that all variables used in ω_w be available.

75. WWPQ(SG,SP,EG,EP,UG,UP,PG,PP,RG,RP,TG,TP,ES,XX,DT,TT,
K1,K2,K3,Z1,Z2,L)

This subroutine calculates the rate of decrease in particle mass per unit volume of mixture due to losses through the duct wall, ω_{wp} .

The only requirement on the terms in the call list is that all variables used in ω_{wp} be available.

76. XINT(A,B,C,D,E)

This subroutine performs linear interpolation using the formula

$$XINT = A + (B-A)E/D.$$

77. VSWICH(L,K1,K2,K3,K4,K5,K6,KK7,KK8,K9,K10)

This subroutine controls the switching of properties from one location to another.

The terms in the call list are:

K1 = first point to be switched
K2 = last " " " "
K3 = 1 always
K4,K5 = properties will be switched from line K5
to line K4.
KG = 1 K7 and K8 = I ($K1 \leq I \leq K2$)
= 2 K7 and K8 = KK7 and KK8
K7,K8 = point K8 will be switched to K7 location
KK7,KK8 = (see K6 = 2)
K9 = 1 always
K10 = 0 always

III. Description of the options available for a user which require subroutines to be altered

1. Change the equation of state

a. To change the equation of state the user must put the equation of state in the following form:

$$p = p(\rho, T)$$

and he must develop relations of the form:

$$f(E, \rho, T) = 0$$

and

$$g(S, \rho, T) = 0$$

b. Subroutines PTQ, QET, NTROPY and FRET must be changed in accordance with the instructions listed in the program.

2. Change the expression for the regression rate

The user must alter subroutine DZDTQ in accordance with instructions in the program.

3. Change the shape of the particles.

The user must change the expressions for the volume of the particle VP as a function of regression distance zz and its time derivative in subroutine QGQ and WGQ.

4. Change the drag force expression.

The user must alter subroutine FQ in accordance with instructions listed in the program.

5. Change the expression for heat transfer with the wall.

The user must alter subroutine QWGQ for the gas phase and QWPQ for the particle phase in accordance with instructions listed in the program.

6. Change the expression for mass transfer with the wall.

The user must alter subroutine WWGQ for the gas phase and WWPQ for the particle phase in accordance with instructions listed in the program.

7. Change the expression for the friction force at the wall.

The user must alter subroutine FWGQ for the gas phase and FWPQ for the particle phase in accordance with instructions listed in the program.

8. Change the expression for the area of the duct as a function of x.

The user must alter subroutines AR and ARX in accordance with the instructions listed in the program.

9. Change the expression for C_v .

The user must alter subroutine SPPT by changing the expression for CV.

IV Instructions for running the computer code TWOFLO (additional information can be found in the sample output, Sec.(6))

1. Before proceeding to discuss the input cards necessary to run TWOFLO, let us first explain the restart option available to the user. This program is designed to allow the user to divide a long run up into several shorter ones, or to extend a run that has been terminated due to process time limits. The important point to be noted is that the data is dumped out by subroutine AOUT and read back into the program in identical format in subroutine AIN. If one wishes to change to a form of output other than a dump file, (ie, punch cards, etc.) his only concern need be that all data currently being transferred out of the program in the present form be transferred out in the new form. This data must then be read back into the program in entirety.

The procedure for utilizing the restart capability when running TWOFLO is as follows:

- a. Define three disk or tape files.
- b. Set KDUMPN = 1 (data is read in from card deck) for initial run and KDUMPN = 2 (data is read in from a file) for subsequent restarts.
- c. Set KDUMPT = 2 (data will be dumped on file for all time lines evenly divisible by NOUTF).
- d. Set the file codes IFILE1, IFILE1, IFILE2 and IFILE3. The data will be read into the program from IFILE1 and immediately dumped on IFILE3 for storage. Subsequent time lines are dumped on both IFILE2 and IFILE3 in accordance with NOUTF.

2. The following is a detailed description of the data cards needed to initiate a calculation using TWOFLO.

VARIABLE NAME	CARD No.	COLUMN No.	FORMAT	DESCRIPTION
KPLOT	1	1-4	I4	= 0 (no plots will be made) = 1 (plots of prescribed variables vs. position will be made.
NPLOTS		5-8	I4	no. of variables to be plotted. It is possible to plot up to six variables vs. position.
NPLOTP		9-12	I4	Every time line divisible by NPLOTP will be plotted.
If KPLOT = 0 omit cards no. 2,3 and 4				
IPLLOT6	2	1-4	I4	= 0 (No plotting) = 1 (plots will be made)
IVARPL(I) I=1,NPLOTS	3	1-4 5-8 9-12 etc.	10I4	Code indicating which variables are to be plotted. (See subroutine INIT for variable codes)
MULT(T) I=1,NPOTS	4	1-4 5-8 9-12 etc,	10I4	Nos. of plots of a particular variable per graph
NOADDB	5	1-4	I4	= 0 Program will automatically add points behind the bullet if required.
NOADDA		5-8	I4	= 1 No pts. will be added behind the bullet
NOADDI		9-12	I4	= 0 Program will automatically add points in front of the bullet if required. = 1 No pts. will be added in front of the bullet. DTMAX before interface is NOADDI times as large as normal
MAXPT	6	1-4	I4	Maximum no. of pts. allowed behind the bullet
MAXPTB		5-8	I4	Maximum no. of pts. allowed in front of bullet.

VARIABLE NAME	CARD No.	COLUMN No.	FORMAT	DESCRIPTION
PTES	7	1-15	E15.8	Limiting value for volume fraction of particles, ϵ . If ϵ at any point is less than PTES particle effects are ignored.
NTCAL	8	1-4	I4	No. of special times lines at which the properties will be interpolated for and printed out. (up to five special times allowable).
If NTCAL = 0 omit card No. 9				
TCAL(I) I=1,NTCAL	9	1-75	5E15.8	The special times at which the properties will be printed out.
KDUMPN	10	1	I1	= 1 (If KDUMPN = 2 data is to be read in from existing disk or tape file. See next section for explanation of input)
KDUMPT		2	I1	= 1 if calculations are not to be dumped on a file = 2 if calculations are to be dumped on existing disk or tape file.
IFILE1		3	I1	If KDUMPT = 1, the values of IFILE1 and IFILE2 are meaningless (set equal to zero) If KDUMPT = 2 calculated time lines are dumped on disk or tape files nos. IFILE2 and IFILE2.
IFILE2		4	I1	
IFILE3		5	I1	If KDUMPN = 1 value of IFILE3 is meaningless (set equal to zero). If KDUMPN = 2 the calculations read in from IFILE1 are dumped on IFILE3 as an auxiliary file
IFILEI		5	I1	If KDUMPN = 2 Initial time line is read in from IFILEI. If KDUMPN = 1 value of IFILEI is meaningless (set equal to zero)

NOUTF	11	1	I1	Any time line number into which NOUTF divides evenly will be dumped on IFILE1 and IFILE2.
NOUTP		2	I1	Any time line into which NOUTP divides evenly will be printed out.
IDRAG	12	1	I1	<div> <div>0 The drag force between particle and gas phases is set equal to zero.</div> <div>1 Drag force is calculated.</div> </div>
B-CONSTANTS	13-42	1-60	4E15.8	On the next thirty(30) cards the B-CONSTANTS are read in, four(4) values per card (a total of 120 CONSTANTS) Card No. eleven(11) would contain B(1,1), B(1,2), B(1,3), and B(1,4) card twelve B(1,5), B(1,6), B(1,7) B(1,8) card No. 26 B(2,1), B(2,2) B(2,3), B(2,4) etc. (a description of the b CONSTANTS appears at the end of this section).
PERPGD	43	1-15	E15.8	.50000000E-02
PERUGD		16-30	E15.8	.50000000E-02
PERRGD		31-45	E15.8	.50000000E-02
PERPGA	44	1-15	E15.8	.10000000E-02
PERUGA		16-30	E15.8	.10000000E-02
PERRGA		31-45	E15.8	.10000000E-02
TIME	45	1-15	E15.8	The time of the initial time line
NTIME		16-19	I4	Time line number of the initial time line
NDELT		20-23	I4	No. of time lines to be calculated
TMAX		24-38	E15.8	Time of last time line calculated will be less than TMAX (This parameter overrides NDELT)

DTMIN	46	1-15	E15.8	The minimum value for DELTA t (time)
DTMAX		16-30	E15.8	The maximum value for DELTA t
DTFIX		31-45	E15.8	If calculated value of DT is greater than DTFIX, DT will be set equal to DTFIX without adding points
MAXIT	47	1-4	I4	Maximum number of iterations
PXTOL	48	1-15	E15.8	If pressure gradient between two successive points on time line is greater than PXTOL and ISMAX > 0, a shock is inserted
NDISC	49	1-4	I4	0 number of area discontinuities (not including gas-particle interface) in the problem
If NDISC = 0 omit card No. 50				
IDISC(KA)	50	1-4	10I4	The point numbers of the area discontinuities
IFRE(1)	51	1-4	I4	Point number of breech
IFRE(2)		5-8	I4	Point number of left surface of bullet
INT(1)		9-12	I4	Point number of interface between gas and two-phase region
IFRE(3)		13-16	I4	Point number of right surface of bullet
IFRE(4)		17-20	I4	Point number of muzzle
TOLSG	52	1-15	E15.8	The following twelve variables are the tolerances used in the program's iterating procedure e.g., TOLSG is the tolerance for SG(gas concentration) see output for further information
TOLEG		16-30	E15.8	
TOLUG		31-45	E15.8	
TOLPG		46-60	E15.8	
TOLRG		61-75	E15.8	
TOLSP	53	1-15	E15.8	
TOLEP		16-30	E15.8	
TOLUP		31-45	E15.8	
TOLPP		46-60	E15.8	
TOLEP		61-75	E15.8	

TOLES	54	1-15	E15.8	
TOXX		16-30	E15.8	
MEOS(1)	55	1-2	I2	<ul style="list-style-type: none"> = 1 A virial equation of state is used in region behind the bullet = 2 Van der Waals equation of state used in region behind the bullet = 3 Noble-Abel equation of state is used in region behind the bullet
MEOS(2)		3-4	I2	= 1,2 or 3 same as MEOS(1) except region is in front of the bullet.
ISMAX	56	1-4	I4	= number of shocks initially inserted (<2)
If ISMAX = 0 omit cards No. 57 and 58.				
IS(1)	57	1-4	I4	point number where shock number 1 is to be inserted.
ISRIL2(1)		5-8	I4	<ul style="list-style-type: none"> = 1 right traveling shock is inserted = 2 left traveling shock is inserted
PGSH(1)		9-23	E15.8	pressure behind the shock
If ISMAX = 1 omit card No. 58				
IS(2)	58	1-4	I4	point number where shock number 2 is to be inserted (must be in front of bullet)
ISRIL2(2)		5-8	I4	<ul style="list-style-type: none"> = 1 right traveling shock is inserted. = 2 left traveling shock is inserted
PGSH(2)		9-23	E15.8	pressure behind the shock
LCODE	59	1-4	I4	= 1 Properties of all pts. behind bullet are initially the same. There will be IFRE(2) -1 such pts., each separated by a DELTA X of DX (calculated in subroutine INIT) only one set of properties behind bullet should be read in

LCODEB		5-8	I4	<ul style="list-style-type: none"> = 0 Properties of all pts. behind bullet must be read in = 1 Properties of all pts. in front of the bullet are initially the same. There will be IFRE(4)-IFRE(3)-1 such pts., each being separated by a DELTA X of (calculated in INIT) only one set of properties in front of bullet should be read in. = 0 Properties of all pts. in front of bullet must be read in.
<p>If LCODE = 1 one set of cards 60-62 should be read in</p> <p>= 2 IFRE(2) sets of cards 60-62 should be read in</p>				
IK	60	1-4	I4	=1
IJ		5-8	I4	Point number of properties on initial time line
XX(1,I)		9-23	E15.8	Distance from IFRE(1) on initial time line.
UG(1,I)		24-38	E15.8	Gas velocity
RG(1,I)		39-53		Gas density
PG(1,I)		54-68	E15.8	Gas pressure
If IJ > INT(1) do not read cards 61 and 62				
UP(1,I)	61	1-15	E15.8	Particle velocity
EP(1,I)		16-30	E15.8	= 0.0
RP(1,I)		31-45	E15.8	Particle density
ES(1,I)		46-60		Volume fraction of particles
ZZ(1,I)	62	1-15	E15.3	Regression distance
<p>If LCODEB = 1 and IFRE(4) ≠ IFRE(2) read card 63</p> <p>= 2 and " " " " " " " " IFRE(4)-IFRE(2) times</p>				
Same as card 60	63			

NODIM	64	1-4	I4	- 1 Causes nondimensionalization - 0 No nondimensionalization
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3. The following data cards are used to restart TWOFL0

VARIABLE NAME	CARD No.	COLUMN No.	FORMAT	DESCRIPTION
<p>The following data cards are used to restart the program.</p> <p>Cards 1-9 are the same as the initial data</p> <p>Card 10 is the same as the initial data except KDUMP=2</p> <p>Cards 11-12 are the same as the initial data</p> <p>Cards 13-15 are the same as card 52-54 in the initial data</p>				
TMAX	16	1-15	E15.8	time of last time line calculated will be less than TMAX (this parameter overrides NDEL T).
NDTNEW	17	1	I1	- 1 Value of DELTA T remains the same (no change for restart)
DTNEW		2-16	E15.8	- 2 Value of DELTA T is set equal to DTNEW If NDTNEW = 1, value of DTNEW is meaningless (set equal to zero) If NDTNEW = 2, DELTA T is set equal to DTNEW
NDTMIN		17	I1	- 1 Value of DTMIN (see previous section for explanation) remains same
DTMINW		18-32	E15.8	- 2 DTMIN is set equal to DTMINW If NDTMIN = 1, value of DTMINW is meaningless (set equal to zero) If NDTMIN = 2, DTMIN is set equal to DTMINW
NDEL T		33-36	I4	The number of time lines to be calculated on this run.
NDTFIX		37-40	I4	- 1 Value of DTFIX remains same. - 2 Value of DTFIX is set equal to DTFIXW

DTFIXW		41-55	E15.8	<p>If NDTFIX = 1, value of DTFIXW is meaningless (set equal to zero)</p> <p>If NDTFIX = 2, DTFIX is set equal to DTFIXW.</p>
NDTMAX	18	1	I1	<p>1, Value of DTMAX remains the same.</p> <p>2 Value of DTMAX is changed to DTMAXW</p>
DTMAXW		2-16	E15.8	<p>If NDTMAX = 1, value of DTMAXW is meaningless (set equal to zero)</p> <p>If NDTMAX = 2, DTMAX is set equal to DTMAXW</p>
NINT	19	1	I1	<p>1, Value of INT(1) remains the same</p> <p>2, Value of INT(2) is set equal to INTW</p>
INTW		2-4	I3	<p>If NINT = 1, Value of INTW is meaningless (set equal to zero)</p> <p>If NINT = 2, Value of INT(1) is set equal to INTW</p>
NPXTOL	20	1-4	I4	<p>1, Value of PXTOL remains the same</p> <p>2, Value of PXTOL is set equal to PXTOLW (If ϵ is less than PXTOL particle properties are ignored)</p>
PXTOLW		5-19	E15.8	<p>If NPXTOL = 1 value of PXTOLW is meaningless (set equal to zero)</p> <p>If NPXTOL = 2, PXTOL is set equal to PXTOLW.</p>

4. Description of the B(2,60) array input constants.

The "B" constants which specify material properties will be underlined. Such properties designated by the 1 location in the array (ie. B(1,)) are for the material behind the bullet; while those designated by the 2 location are for the material in front of the bullet. Thus it is only necessary to explain the B(1,) portion of the array. Any constants that are not explained below are currently not defined in the code and can be set equal to zero.

<u>B(1,1)</u>	= ρ_0 , Reference density for Equation of State.
<u>B(1,2)</u>	= T_0 , Reference temperature for Equation of State.
<u>B(1,3)</u>	= E_0 , Reference energy for the Equation of State.
<u>B(1,4)</u>	= p_0 , Reference pressure for Equation of State.
<u>B(1,5)</u>	= Geometrical parameter used in subroutines QGQ and WGQ to describe the particle shape.
B(1,6)	= Geometrical parameter used in subroutines QGQ and WGQ to describe the particle shape.
B(1,8)	= p_h , Hold back pressure
<u>B(1,11)</u>	= R , Universal gas constant
<u>B(1,12)</u>	= M , Mass of gas per mole
<u>B(1,13)</u>	= Constant in Van der Waal Equation of State
<u>B(1,14)</u>	= Constant in Van der Waal Equation of State
<u>B(1,17)</u>	= T_w , Wall temperature
B(1,20)	= ρ_d , Nondimensionalizing density
B(1,21)	= x_d , Nondimensionalizing distance
B(1,22)	= p_d , Nondimensionalizing pressure
B(1,23)	= Initial x location of the bullet
B(1,24)	= L_B , Bullet length
B(1,25)	= L_{BR} , Barrel length (measured from the beginning of the barrel diameter)
B(1,26)	= D , Diameter of the chamber
B(1,27)	= x^c , x location where chamber diameter ends
B(1,28)	= D_B , Barrel diameter
B(1,29)	= x_B , x location of the beginning of the barrel diameter
B(1,30)	= μ_0 , Reference dynamic viscosity used to calculate μ
B(1,31)	= Reference temperature used to calculate μ
B(1,32)	= Reference pressure used to calculate μ
B(1,33)	= Constant used to calculate μ
B(1,34)	= Constant used to calculate μ
B(1,35)	= K , Particle velocity ratio across area discontinuity
B(1,36)	= T_m , Reference temperature used in entropy equation
<u>B(1,37)</u>	= A_1 , Constant in equation for C_v
<u>B(1,38)</u>	= A_2 , Constant in equation for C_p
<u>B(1,40)</u>	= \bar{E}^2 , Specific internal energy of combustion products
B(1,41)	= K_Q , Heat released per unit volume of propellant burnt
B(1,42)	= α_Q , Constant in regression formula
B(1,43)	= β , Constant in regression formula

B(1,48) = F_R , Bore resistance force
 B(1,49) = A_B , Cross-sectional area of the bullet
 B(1,50) = M_B , Bullet mass
 B(1,51) = p_M , Muzzle pressure
 B(1,52) = t_{SD} , The time that it takes for p_{EXIT} to reach p_M
 after the shock leaves the barrel
 B(1,53) = t_{BD} , The time that it takes for p_{BEX} to reach p_M
 after the bullet leaves the barrel

5. Description of user specified functions and variables currently in TWOFLO.

a. Drag Force (spherical particle)

$$F = \frac{3}{8} CD \cdot \epsilon \cdot \rho \cdot |u - u_p| \cdot (u - u_p) / B(1,5)$$

where

$$CD = \frac{24}{RE} + 4 \cdot RE^{-1/3}$$

$$RE = 2 \cdot \rho \cdot B(1,5) \cdot |u - u_p| / \mu$$

$$\mu = B(1,30) + [T - B(1,31)] \cdot B(1,33) + [p - B(1,32)] \cdot B(1,34)$$

b. Constant volume specific heat C_v

$$C_v = B(L,37) + B(L,38) \cdot T \quad (L=1,2)$$

c. Equation of State (Ideal gas)

$$p = B(L,11) \cdot \rho \cdot T / B(L,12) \quad (L=1,2)$$

d. Volume of a particle (pancake)

$$V_p = \pi \cdot [B(1,5) - Z]^2 \cdot \{B(1,6) + 4 \cdot [B(1,5) - Z] / 3\}$$

e. Various parameters in Eq. (3)

$$\phi = F u_p / \sigma$$

$$u_w = u$$

$$v_w = 0$$

$$E_w = E$$

$$p_w = p$$

$$\rho_w = \rho$$

6. Sample initial data

The sample input data presented here correspondes to computer runs A,B and C presented in the Results and Conclusions section of the main report.

```
CARD 1  KPLOT      = 0
        NPLOTS     = 0
        NPLOTP     = 0

CARD 2  Not used*  (omit this card)

CARD 3  Not used  (omit this card)

CARD 4  Not used  (omit this card)

CARD 5  NOADDB     = 0
        NOADDA     = 1
        NOADDI     = 3

CARD 6  MAXPT      = 30
        MAXPTB     = Not used (an arbitrary value of 0 is read in)

CARD 7  PTE$      = 0.10000000E-02

CARD 8  NTCAL      = 4

CARD 9  TCAL(1)    = 0.20000000E-03 s
        TCAL(2)    = 0.40000000E-03 s
        TCAL(3)    = 0.60000000E-03 s
        TCAL(4)    = 0.80000000E-03 s

CARD 10 KDUMPN     = 1
        KDUMPT     = 2
        IFILE1     = 1
        IFILE2     = 2
        IFILE3     = 1
        IFILEI     = 1

CARD 11 NOUTF      = 1
        NOUTP      = 1

CARD 12 IDRAG      = 1

CARD 13 B(1,1)     = 0.12800000E+01 kg/m3
        B(1,2)     = Not used (an arbitrary value of 0.0 K is read in)
        B(1,3)     = Not used (an arbitrary value of 0.0 J/kg is read in)
        B(1,4)     = Not used (an arbitrary value of 0.0 Pa is read in)

CARD 14 B(1,5)     = 0.27305000E-03 m (Runs A & C) 0.13650000E-03 m (Run C)
        B(1,6)     = 0.38100000E-03 m (Runs A & C) 0.19050000E-03 m (Run C)
        B(1,7)     = Not defined**
        B(1,8)     = 0.20700000E+08 Pa
```

* The term Not used indicates that the variable is defined but not used for this specific run.

**The term Not defined indicates that the term is never used in the program.

CARD 15 B(1,9) = Not defined = 0.00000000E+00
 B(1,10) = Not defined = 0.00000000E+00
 B(1,11) = 0.83140000E+01 J/(K·mol)
 B(1,12) = 0.25547800E-01 kg/mol

CARD 16 B(1,13) = Not used (an arbitrary value of 0.0 N·m⁶/kg² is read in)
 B(1,14) = Not used (an arbitrary value of 0.0 m³/kg is read in)
 B(1,15) = Not defined = 0.00000000E+00
 B(1,16) = Not defined = 0.00000000E+00

CARD 17 B(1,17) = 0.00000000E+00 K
 B(1,18) = Not defined = 0.00000000E+00
 B(1,19) = Not defined = 0.00000000E+00
 B(1,20) = 0.15000000E+03 kg/m³

CARD 18 B(1,21) = 0.40000000E-01 m
 B(1,22) = 0.20000000E+09 Pa
 B(1,23) = 0.33100000E-01 m
 B(1,24) = 0.15000000E-01 m

CARD 19 B(1,25) = 0.47000000E+00 m
 B(1,26) = 0.90750000E-02 m
 B(1,27) = 0.26850000E-01 m
 B(1,28) = 0.56500000E-02 m

CARD 20 B(1,29) = 0.31000000E-01 m
 B(1,30) = 0.18192000E-04 N·s/m²
 B(1,31) = 0.29300000E+03 K
 B(1,32) = 0.10130000E+06 Pa

CARD 21 B(1,33) = 0.53600000E-07 N·s/(m²·K)
 B(1,34) = 0.12080000E-12 s
 B(1,35) = Not defined = 0.00000000E+00
 B(1,36) = 0.29800000E+03 K

CARD 22 B(1,37) = 0.13559000E+04 J/(kg·K)
 B(1,38) = 0.00000000E+00 J/(kg·K²)
 B(1,39) = Not defined = 0.00000000E+00
 B(1,40) = 0.00000000E+00 J/kg

CARD 23 B(1,41) = 0.63000000E+10 J/m³
 B(1,42) = 0.12000000E-07 m/(Pa^β·s) (β=B(1,43))
 B(1,43) = 0.84550000E+00
 B(1,44) = Not defined = 0.00000000E+00

CARD 24 B(1,45) = Not defined = 0.00000000E+00
 B(1,46) = Not defined = 0.00000000E+00
 B(1,47) = Not defined = 0.00000000E+00
 B(1,48) = 0.16700000E+03 N

CARD 25 B(1,49) = 0.24279500E-04 m²
 B(1,50) = 0.36290000E-02 kg
 B(1,51) = 0.10132500E+06 Pa
 B(1,52) = 0.20000000E-04 s

 CARD 26 B(1,53) = 0.50000000E-04 s
 B(1,54) = Not defined = 0.00000000E+00
 B(1,55) = Not defined = 0.00000000E+00
 B(1,56) = Not defined = 0.00000000E+00

 CARD 27 B(1,57) - B(1,60) = Not defined = 0.00000000E+00

 CARD 28 B(2,1) = Not used (an arbitrary value of 0.0 kg/m³ is read in)
 B(2,2) = Not used (an arbitrary value of 0.0 K is read in)
 B(2,3) = Not used (an arbitrary value of 0.0 J/kg is read in)
 B(2,4) = Not used (an arbitrary value of 0.0 Pa is read in)

 CARD 29 B(2,5) - B(2,8) = Not defined = 0.00000000E+00

 CARD 30 B(2,9) = Not defined = 0.00000000E+00
 B(2,10) = Not defined = 0.00000000E+00
 B(2,11) = Not used (an arbitrary value of 0.0 J/(K·mol) is read in)
 B(2,12) = Not used (an arbitrary value of 0.0 kg/mol is read in)

 CARD 31 B(2,13) = Not used (an arbitrary value of 0.0 N·m⁶/kg² is read in)
 B(2,14) = Not used (an arbitrary value of 0.0 m³/kg is read in)
 B(2,15) = Not defined = 0.00000000E+00
 B(2,16) = Not defined = 0.00000000E+00

 CARD 32 B(2,17) - B(2,20) = Not defined = 0.00000000E+00

 CARD 33 B(2,21) - B(2,24) = Not defined = 0.00000000E+00

 CARD 34 B(2,25) - B(2,28) = Not defined = 0.00000000E+00

 CARD 35 B(2,29) - B(2,32) = Not defined = 0.00000000E+00

 CARD 36 B(2,33) = Not defined = 0.00000000E+00
 B(2,34) = Not defined = 0.00000000E+00
 B(2,35) = Not defined = 0.00000000E+00
 B(2,36) = Not used (an arbitrary value of 0.0 K is read in)

 CARD 37 B(2,37) = Not used (an arbitrary value of 0.0 J/(kg·K) is read in)
 B(2,38) = Not used (an arbitrary value of 0.0 J/(kg·K²) is read in)
 B(2,39) = Not defined = 0.00000000E+00
 B(2,40) = Not defined = 0.00000000E+00

CARD 38 B(2,41) - B(2,44) = Not defined = 0.00000000E+00
 CARD 39 B(2,45) - B(2,48) = Not defined = 0.00000000E+00
 CARD 40 B(2,49) - B(2,52) = Not defined = 0.00000000E+00
 CARD 41 B(2,53) - B(2,56) = Not defined = 0.00000000E+00
 CARD 42 B(2,57) - B(2,60) = Not defined = 0.00000000E+00
 CARD 43 PERPGD = 0.50000000E-02
 PERUGD = 0.50000000E-02
 PERRGD = 0.50000000E-02
 CARD 44 PERPGA = 0.10000000E-01
 PERUGA = 0.10000000E-01
 PERRGA = 0.10000000E-01
 CARD 45 TIME = 0.00000000E+00 s
 NTIME = 0
 NDEL T = 40
 TMAX = 0.12000000E-02 s
 CARD 46 DTMIN = 0.45000000E-05 s
 DTMAX = Not used (a value less than 2.2 x DTMIN should
 be read in) = 0.00000000E+00 s
 DTFIX = Not used (a value much larger than DTMIN should
 be read in) = 0.10000000E+10 s
 CARD 47 MAXIT = 15
 CARD 48 PXTOL = 0.50000000E+01 Pa/m
 CARD 49 NDISC = 0 (Program is currently not operational for
 NDISC greater than 0)
 CARD 50 Not used (omit this card)
 CARD 51 IFRE(1) = 1
 IFRE(2) = 6
 INT(1) = 6
 IFRE(3) = 6
 IFRE(4) = 6
 CARD 52 TOLSG = 0.10000000E-02
 TOLEG = 0.10000000E-02
 TOLUG = 0.10000000E-02
 TOLPG = 0.10000000E-02
 TOLRG = 0.10000000E-02

CARD 53 TOLSP = 0.10000000E-02
 TOLEP = Not used (an arbitrary value of 0.10000000E-02
 is read in)
 TOLUP = 0.10000000E-02
 TOLPP = Not used (an arbitrary value of 0.10000000E-02
 is read in)
 TOLRP = Not used (an arbitrary value of 0.10000000E-02
 is read in)

CARD 54 TOLES = 0.10000000E-02
 TOLXX = 0.10000000E-02

CARD 55 MEOS(1) = 3
 MEOS(2) = Not used (an arbitrary value of 3 is read in)

CARD 56 ISMAX = 0

CARD 57 Not used (omit this card)

CARD 58 Not used (omit this card)

CARD 59 LCODE = 1
 LCODEB = Not used (an arbitrary value of 1 is read in)

CARD 60 IK = 1
 IJ = 1
 XX(1,1) = 0.00000000E+00 m
 UG(1,1) = 0.00000000E+00 m/s
 RG(1,1) = 0.10755000E+00 kg/m³ (Runs A & B)
 = 0.14637200E+02 kg/m³ (Run C)
 PG(1,1) = 0.10132500E+06 Pa (Runs A & B)
 = 0.13790000E+08 Pa (Run C)

CARD 61 UP(1,1) = 0.00000000E+00 m/s
 EP(1,1) = Not used (an arbitrary value of 0.00000000E+00 J/kg
 is read in)
 RP(1,1) = 0.16050000E+04 kg/m³
 ES(1,1) = 0.57500000E+00

CARD 62 ZZ(1,1) = 0.00000000E+00 m

CARD 63 Not used (omit this card)

CARD 64 NODIM = 0

	TOLPP	= Not used (an arbitrary value of 0.10000000E-02 is read in)
	TOLRP	= Not used (an arbitrary value of 0.10000000E-02 is read in)
CARD 15	TOLES	= 0.10000000E-02
	TOLXX	= 0.10000000E-02
CARD 16	TMAX	= 0.12000000E-02 s
CARD 17	NDTNEW	= 1
	DTNEW	= Not used (an arbitrary value of 0.00000000E+00 s is read in)
	NDTMIN	= 1
	DTMINW	= Not used (an arbitrary value of 0.00000000E+00 s is read in)
	NDELT	= 5
	NDTFIX	= 1
	DTFIXW	= Not used (an arbitrary value of 0.00000000E+00 s is read in)
CARD 18	NDTMAX	= 1
	DTMAXW	= Not used (an arbitrary value of 0.00000000E+00 s is read in)
CARD 19	NINT	= 1
	INTW	= Not used (an arbitrary value of 0 is read in)
CARD 20	NPXTOL	= 1
	PXTOLW	= Not used (an arbitrary value of 0.00000000E+00 Pa is read in)

7. Sample restart data

CARD 1	KPLOT	=	0
	NPLOTS	=	0
	NPLOTP	=	0
CARD 2	Not used (omit this card)		
CARD 3	Not used (omit this card)		
CARD 4	Not used (omit this card)		
CARD 5	NOADDB	=	0
	NOADDA	=	1
	NOADDI	=	3
CARD 6	MAXPT	=	30
	MAXPTB	=	Not used (an arbitrary value of 0 is read in)
CARD 7	PTES	=	0.10000000E-02
CARD 8	NTCAL	=	4
CARD 9	TCAL(1)	=	0.20000000E-03 s
	TCAL(2)	=	0.40000000E-03 s
	TCAL(3)	=	0.60000000E-03 s
	TCAL(4)	=	0.80000000E-03 s
CARD 10	KDUMPN	=	2
	KDUMPT	=	2
	IFILE1	=	
	IFILE2	=	
	IFILE3	=	
	IFILEI	=	
CARD 11	NOUTF	=	1
	NOUTP	=	1
CARD 12	IDRAC	=	1
CARD 13	TOLSG	=	0.10000000E-02
	TOLEG	=	0.10000000E-02
	TOLUG	=	0.10000000E-02
	TOLPG	=	0.10000000E-02
	TOLRG	=	0.10000000E-02
CARD 14	TOLSP	=	0.10000000E-02
	TOLEP	=	Not used (an arbitrary value of 0.10000000E-02 is read in)
	TOLUP	=	0.10000000E-02

8. Sample initial output

NOMENCLATURE

SG=GAS CONCENTRATION ES=VOL. FRACTION OF PARTICLES RP=PARTICLE DENSITY
 XX=DISTANCE UG=GAS PRESSURE TG=GAS TEMPERATURE
 EG=GAS SPECIFIC INT ENERGY CG=GAS SOUND SPEED TG=GAS TEMPERATURE
 UP=PARTICLE VELOCITY UPX=PARTIAL DERIVATIVE UP,X UPT=PARTIAL DERIVATIVE UP,T
 SP=PARTIAL DERIVATIVE SP,T

KPLOT = 0 MPLOTS = -0 MPLOT = -0

NOADUB = 0
 NOADUA = 1
 NUADUI = 3

IF NUADUB = 1, NU POINTS WILL BE ADDED BEHIND THE BULLET
 IF NUADUA = 1, NU POINTS WILL BE ADDED IN FRONT OF THE BULLET
 NUADUI = 0 MAX. NO. OF PTS. ALLOWED BEHIND THE BULLET

MAXP = 30 MAX. NO. OF PTS. ALLOWED BEHIND THE BULLET
 MAXPB = 0 MAX. NO. OF PTS. ALLOWED IN FRONT OF THE BULLET

PTES = .1000000E-02 (IF ES IS LESS THAN PTES, POINT IS CONSIDERED TO BE GAS-ONLY - PARTICLE EFFECTS IGNORED)

THE NO. OF SPECIAL TIME LINES TO BE CALCULATED(NITCAL) = 4
 THE TIMES OF THESE TIME LINES ARE AS FOLLOWS .2000000E-03 .4000000E-03 .6000000E-03 .8000000E-03

NDUMFN = 1 KOUNTP = 2 IFILE1 = 1 IFILE2 = 2 IFILE3 = 1 IFILE4 = 1
 IF KOUNTPN = 2, TIME LINE WILL BE READ FROM DISK OR TAPE FILE IFILE1.
 IF KOUNTP = 2, CALCULATED TIME LINES WILL BE DUMPED ONTO TAPE OR DISK FILES IFILE1 AND IFILE2.
 AT THE BEGINNING OF EACH RUN, THE TIME LINE HEAD FROM IFILE1 WILL BE STORED UN IFILE3 AS A BACKUP FILE.

NUOTF = 1 ANY TIME LINE INTO WHICH NUOTF DIVIDES EVENLY WILL BE DUMPED ON FILES 1 2
 NUOTP = 1 ANY TIME LINE INTO WHICH NUOTP DIVIDES EVENLY WILL BE PRINTED

IDRAG = 1 IF IDRAG = 0 THERE IS NO DRAG FORCE

THESE ARE CONSTANTS USED IN CRITERIA FOR ADDING AND DROPPING MESH PTS. IN PLANNING.
 PMPGUB = .5000000E-02 PERGUB = .5000000E-02 PERGUB = .5000000E-02
 PLRPUA = .1000000E 00 PERPUA = .1000000E 00 PERPUA = .1000000E 00

THE TIME OF THE INITIAL TIME PLANE (TIME) IS .0
 THE TIME PLANE NUMBER OF THE INITIAL TIME PLANE (NTIME) IS 0
 THE NUMBER OF TIME PLANES TO BE CALCULATED (NDELTA) IS 100
 THE NUMBER OF THE LAST TIME PLANE TO BE CALCULATED (NTIME) IS 100
 THE TIME OF THE LAST TIME LINE CALCULATED ON THIS RUN WILL BE LESS THAN (TIME) .1200000E-02 (THIS PARAMETER OVERRIDES NDELTA)

THE MAXIMUM VALUE FOR DELTA T (DTMAX) IS .0
 THE MINIMUM VALUE FOR DELTA T (DTMIN) IS .4500000E-05

UTFIX = .1000000E 10 IF THE CALCULATED UT IS GREATER THAN UFIX, UT WILL BE SET EQUAL TO UFIX, BUT NO NEW POINTS WILL BE ADDED.

MAXIT = 15 MAX. NO. OF ITERATIONS USED

PXTOL = .5000000E 01
 IF PRESSURE GRADIENT BETWEEN TWO SUCCESSIVE POINTS ON TIME LINE IS GREATER THAN PXTOL,
 AND CHARACTERISTICS OF THE SAME FAMILY CROSS, A SHOCK IS INSERTED.

NOISC = 0
 NOISC IS THE NOS. OF AREA DISCONTINUITIES (NOT INCLUDING GAS-PARTICLE INTERFACE):

IFNE(1) = 1 POINT NOS. OF BREECH
 IFNE(2) = 6 POINT NOS. OF LEFT SURFACE OF MULLET
 IFNE(3) = 6 POINT NOS. OF RIGHT SURFACE OF BULLET
 IFNE(4) = 6 POINT NOS. OF MUZZLE
 INT(1) = 6 POINT NOS. OF INTERFACE BETWEEN GAS AND TWO PHASE REGION
 IF ONE DOES NOT WISH TO CALCULATE THE EFFECTS OF THE GAS IN FRONT OF THE MULLET, HE SHOULD SET IFNE(4) AND IFNE(4) EQUAL TO

THE NUMBER OF POINTS IN THE INITIAL TIME LINE (MXNPT) IS 6

TOLSA	TOLG	TOLUG	TOLPG	TOLRW
.1000000E-02	.1000000E-02	.1000000E-02	.1000000E-02	.1000000E-02
TOLSA	TOLP	TOLUP	TOLPP	TOLRP
.1000000E-02	.1000000E-02	.1000000E-02	.1000000E-02	.1000000E-02

TOLSA
 .1000000E-02
 .1000000E-02

THE TWELVE VARIABLES ABOVE ARE THE TOLERANCES USED IN THE ITERATING PROCEDURES. E.G., TOLPS = TOLERANCE FOR GAS CONCENTRATION.

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9 Sample restart output

NOMENCLATURE

SG=GAS CONCENTRATION
 XX=DISTANCE
 EG=GAS SPECIFIC INT ENERGY
 UP=PARTICLE VELOCITY
 SPT=PARTIAL DERIVATIVE SP.T
 SP=PARTICLE CONCENTRATION
 UG=GAS VELOCITY
 CG=GAS SOUND SPEED
 UPX=PARTIAL DERIVATIVE UP,X
 ES=VD. CT. N OF PARTICLES
 PG=GAS PRESSU
 TG=GAS TEMPERATURE
 UG=PARTIAL DERIVATIVE UP,T
 HP=PARTICLE DENSITY
 TG=GAS TEMPERATURE
 ZZ=REGRESSION DISTANCE
 SPX=PARTIAL DERIVATIVE SP,X

NPLOT = 0 NPLOTS = -0 NPLOT = -0

NUADD = 0
 NUADDL = 1
 NUADDI = 3
 IF NUADD = 1, NO POINTS WILL BE ADDED BEHIND THE BULLET
 IF NUADDL = 1, NO POINTS WILL BE ADDED IN FRONT OF THE BULLET
 NUADDI = 0 MAX. NO. OF PTS. ALLOWED IN FRONT OF THE BULLET

MAXPT = 30 MAX. NO. OF PTS. ALLOWED BEHIND THE BULLET
 MAXPTL = 0 MAX. NO. OF PTS. ALLOWED IN FRONT OF THE BULLET

PTES = .1000000E-02 (IF ES IS LESS THAN PTES, POINT IS CONSIDERED TO BE GAS-ONLY - PARTICLE EFFECTS IGNORED)

THE NO. OF SPECIAL TIME LINES TO BE CALCULATED(NICAL) = 4
 THE TIMES OF THESE TIME LINES ARE AS FOLLOWS .2000000E-03 .4000000E-03 .6000000E-03 .8000000E-03

KOUNPN = 2 KOUNPT = 2 IFILE1 = 2 IFILE2 = 1 IFILE3 = 2 IFILE4 = 2
 IF KOUNPN = 2, TIME LINE WILL BE READ FROM DISK OR TAPE FILE IFILE1.
 IF KOUNPT = 2, CALCULATED TIME LINES WILL BE DUMPED ONTO TAPE OR DISK FILES IFILE1 AND IFILE2.
 AT THE BEGINNING OF EACH RUN, THE TIME LINE HEAD FROM IFILE1 WILL BE STORED ON IFILE3 AS A BACKUP FILE.

NOUTF = 1 ANY TIME LINE INTO WHICH NOUTF DIVIDES EVENLY WILL BE DUMPED ON FILES 2 1
 NOUTP = 1 ANY TIME LINE INTO WHICH NOUTP DIVIDES EVENLY WILL BE PRINTED

IDRAG = 1 IF IDRAG = 0 THERE IS NO DRAG FORCE

B(1, 1) =	.12400000E 01	B(1, 2) =	-.0	B(1, 3) =	-.0	B(1, 4) =	-.0	B(1, 5) =	-.0
B(1, 5) =	.27305000E-03	B(1, 6) =	.36100000E-03	B(1, 7) =	.0	B(1, 8) =	.26700000E 04	B(1, 9) =	.25500000E-01
B(1, 9) =	.0	B(1, 10) =	.12400000E 01	B(1, 11) =	.0	B(1, 12) =	.0	B(1, 13) =	.0
B(1, 13) =	.0	B(1, 14) =	.0	B(1, 15) =	.0	B(1, 16) =	.0	B(1, 17) =	.0
B(1, 17) =	.0	B(1, 18) =	.0	B(1, 19) =	.0	B(1, 20) =	.15000000E 03	B(1, 21) =	.15000000E 03
B(1, 21) =	.40600000E-01	B(1, 22) =	.20000000E 09	B(1, 23) =	.33100000E-01	B(1, 24) =	.15000000E-01	B(1, 25) =	.15000000E-01
B(1, 25) =	.47000000E 00	B(1, 26) =	.90750000E-02	B(1, 27) =	.26850000E-01	B(1, 28) =	.55500000E-02	B(1, 29) =	.55500000E-02
B(1, 29) =	.31000000E-01	B(1, 30) =	.15192000E-04	B(1, 31) =	.0	B(1, 32) =	.15100000E 06	B(1, 33) =	.15100000E 06
B(1, 33) =	.53600000E-07	B(1, 34) =	.12080000E-12	B(1, 35) =	.0	B(1, 36) =	.27800000E 03	B(1, 37) =	.27800000E 03
B(1, 37) =	.13559000E 04	B(1, 38) =	.0	B(1, 39) =	.0	B(1, 40) =	.0	B(1, 41) =	.0
B(1, 41) =	.63000000E 10	B(1, 42) =	.12000000E-07	B(1, 43) =	.0	B(1, 44) =	.0	B(1, 45) =	.0
B(1, 45) =	.0	B(1, 46) =	.0	B(1, 47) =	.0	B(1, 48) =	.16700000E 03	B(1, 49) =	.16700000E 03
B(1, 49) =	.24279500E-04	B(1, 50) =	.36290000E-02	B(1, 51) =	.0	B(1, 52) =	.25000000E-04	B(1, 53) =	.25000000E-04
B(1, 53) =	.50000000E-04	B(1, 54) =	.43000000E-01	B(1, 55) =	.0	B(1, 56) =	.0	B(1, 57) =	.0
B(1, 57) =	.0	B(1, 58) =	.0	B(1, 59) =	.0	B(1, 60) =	.0	B(2, 1) =	.0
B(2, 1) =	.12800000E 01	B(2, 2) =	.0	B(2, 3) =	.0	B(2, 4) =	.0	B(2, 5) =	.0
B(2, 5) =	.0	B(2, 6) =	.0	B(2, 7) =	.0	B(2, 8) =	.0	B(2, 9) =	.0
B(2, 9) =	.0	B(2, 10) =	.12400000E 01	B(2, 11) =	.0	B(2, 12) =	.27800000E-01	B(2, 13) =	.27800000E-01
B(2, 13) =	.0	B(2, 14) =	.0	B(2, 15) =	.0	B(2, 16) =	.0	B(2, 17) =	.0
B(2, 17) =	.0	B(2, 18) =	.0	B(2, 19) =	.0	B(2, 20) =	.0	B(2, 21) =	.0
B(2, 21) =	.0	B(2, 22) =	.0	B(2, 23) =	.0	B(2, 24) =	.0	B(2, 25) =	.0
B(2, 25) =	.0	B(2, 26) =	.0	B(2, 27) =	.0	B(2, 28) =	.0	B(2, 29) =	.0
B(2, 29) =	.0	B(2, 30) =	.0	B(2, 31) =	.0	B(2, 32) =	.0	B(2, 33) =	.0
B(2, 33) =	.0	B(2, 34) =	.0	B(2, 35) =	.0	B(2, 36) =	.0	B(2, 37) =	.0
B(2, 37) =	.13559000E 04	B(2, 38) =	.0	B(2, 39) =	.0	B(2, 40) =	.0	B(2, 41) =	.0
B(2, 41) =	.64400000E 10	B(2, 42) =	.20000000E-06	B(2, 43) =	.90000000E 00	B(2, 44) =	.0	B(2, 45) =	.0
B(2, 45) =	.0	B(2, 46) =	.0	B(2, 47) =	.0	B(2, 48) =	.0	B(2, 49) =	.0
B(2, 49) =	.0	B(2, 50) =	.0	B(2, 51) =	.0	B(2, 52) =	.0	B(2, 53) =	.0
B(2, 53) =	.0	B(2, 54) =	.0	B(2, 55) =	.0	B(2, 56) =	.0	B(2, 57) =	.0
B(2, 57) =	.0	B(2, 58) =	.0	B(2, 59) =	.0	B(2, 60) =	.0		


```

TOLSG      TOLG      TOLPG      TOLMG
.10000000E-02 .1000000E-02 .1000000E-02 .1000000E-02
TOLSP      TOLP      TOLPP      TOLMP
.1000000E-02 .1000000E-02 .1000000E-02 .1000000E-02
TOLX      TOLXX
.1000000E-02 .1000000E-02

```

THE TWELVE VARIABLES ABOVE ARE THE TOLERANCES USED IN THE ITERATING PROCEDURES .E.G., TOLSG - TOLERANCE FOR GAS CONCENTRATION.

THE MAXIMUM TIME FOR CALCULATION IN THIS PROBLEM(TMAX) IS .12000000E-02

```

NCTNEM = 1 DTNEM = .0      NDTMIN = 1 DTMIN = .0      NDEL = 5 NUTFIX = 1 DTFIX = .0
IF NUTNEM = 1 VALUE OF DELTA T REMAINS THE SAME
IF NCTNEM = 2 DELTA T IS SET EQUAL TO DTNEM

```

```

IF NUTMIN = 1 VALUE OF DTMIN STAYS THE SAME
IF NUTMIN = 2 DTMIN IS SET EQUAL TO DTMIN

```

```

IF NUTFIX = 1 VALUE OF DTFIX STAYS THE SAME
IF NUTFIX = 2 DTFIX IS SET EQUAL TO DTFIX

```

NDEL - NUMBER OF TIME LINES TO BE CALCULATED ON THIS RUN

```

NCTMAX = 1 DTMAX = .0
IF NUTMAX = 1 VALUE OF DTMAX STAYS THE SAME
IF NCTMAX = 2 DTMAX IS SET EQUAL TO DTMAX

```

```

NINT = 1 INTN = 0
IF NINT = 1 VALUE OF INT(1) STAYS THE SAME
IF NINT = 2 INT(1) IS SET EQUAL TO INTN

```

NPERUN = 1

APERUN = 1

```

NPXTOL = 1 PXTOLN = .0
IF NPXTOL = 1 VALUE OF PXTOL STAYS THE SAME
IF NPXTOL = 2 PXTOL IS SET EQUAL TO PXTOLN

```


WE HAVE FINISHED READING TIME LINE 40 FROM FILE 2
 THE TIME OF TIME LINE 40 IS .21958600E-03

POINT NO.	XX	UG ZZ UPX	PG UP UPT	KG SU SPA	LG SP SPT	LU LS	TG MP
1	1	.0	.69755018E 00	.73437032E 02	.39575630E 07	.10852770E 04	.29107725E 04
		.0	.0	.32015703E 02	.88780237E 03	.55314707E 00	.16050000E 04
		.0	.0	.63022073E 03	.84810237E 00		
1	2	.71061015E-02	.67600000E 00	.70340395E 02	.40037247E 07	.10915000E 04	.29520172E 04
		.0	.12004070E 01	.31277402E 02	.89140400E 03	.55539192E 00	.16050000E 04
		.0	.60114502E 05	.31656070E 03	.60272190E 06		
1	3	.13670564E-01	.67199419E 00	.70951201E 02	.39461769E 07	.10837154E 04	.29103740E 04
		.0	.97397142E 00	.31499459E 02	.89244563E 03	.55604009E 00	.16050000E 04
		.0	.65460411E 05	.12989931E 02	.51600519E 06		
1	4	.20242135E-01	.66590906E 00	.70496941E 02	.39361167E 07	.10823331E 04	.29029550E 04
		.0	.81532170E 00	.31325002E 02	.89173700E 03	.55559941E 00	.16050000E 04
		.0	.77718063E 05	.91490449E 02	.54638032E 06		
1	5	.26067667E-01	.6565776E 00	.69662103E 02	.39269905E 07	.10810700E 04	.28962302E 04
		.0	.73623033E 00	.30966245E 02	.89154431E 03	.55547934E 00	.16050000E 04
		.0	.64052772E 05	.27419575E 02	.55094300E 06		
1	6	.33109870E-01	.64903535E 00	.69016110E 02	.39182216E 07	.10790700E 04	.28697570E 04
		.0	.80040071E 00	.30691112E 02	.89126475E 03	.55530514E 00	.16050000E 04
		.0	.56249000E 05	.52399902E 02	.56710016E 06		
PGINI NO.	XX	UG ZZ UPX	PG UP UPT	KG SU SPA	LG SP SPT	LU LS	TG MP
1	7	.33109870E-01	.64917537E 00	.69020123E 02	.39183852E 07	.10790725E 04	.28698777E 04
1	8	.33371691E-01	.64504790E 00	.56200240E 02	.47821693E 07	.11929973E 04	.35209330E 04
INT(1) =	6	IFRE(1) =	1	IFRE(2) =	1		
IFRE(3) =	8	IFRE(4) =	8				

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